# Package 'rawrr'

July 28, 2025

**Type** Package

**Title** Direct Access to Orbitrap Data and Beyond

**Version** 1.16.0

**Depends** R (>= 4.1)

**Imports** grDevices, graphics, stats, utils

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

**Description** This package wraps the functionality of the Thermo Fisher Scientic RawFileReader .NET 8.0 assembly. Within the R environment, spectra and chromatograms are represented by S3 objects. The package provides basic functions to download and install the required third-party libraries. The package is developed, tested, and used at the Functional Genomics Center Zurich, Switzerland.

**License** GPL-3

**SystemRequirements** .NET 8.0 (optional; required only if you want to compile and link the C# code)

**URL** https://github.com/fgcz/rawrr/

**BugReports** https://github.com/fgcz/rawrr/issues

**Encoding** UTF-8

**NeedsCompilation** no

**RoxygenNote** 7.3.2

**biocViews** MassSpectrometry, Proteomics, Metabolomics, Infrastructure, Software

**VignetteBuilder** knitr

**git_url** https://git.bioconductor.org/packages/rawrr

**git_branch** RELEASE_3_21

**git_last_commit** 9604ecc

**git_last_commit_date** 2025-04-15

**Repository** Bioconductor 3.21

**Date/Publication** 2025-07-27

**Author** Christian Panse [aut, cre] (ORCID:
<https://orcid.org/0000-0003-1975-3064>),
Leonardo Schwarz [ctb] (ORCID: <https://orcid.org/0009-0003-1828-6924>),
Tobias Kockmann [aut] (ORCID: <https://orcid.org/0000-0002-1847-885X>)

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

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`rawrr-package` *rawrr: Direct Access to Orbitrap Data and Beyond*

---

## Description

This package wraps the functionality of the Thermo Fisher Scientic RawFileReader .NET 8.0 assembly. Within the R environment, spectra and chromatograms are represented by S3 objects. The package provides basic functions to download and install the required third-party libraries. The package is developed, tested, and used at the Functional Genomics Center Zurich, Switzerland.

## Author(s)

**Maintainer**: Christian Panse <cp@fgcz.ethz.ch> (ORCID)

Authors:

- Tobias Kockmann <tobias.kockmann@fgcz.ethz.ch> (ORCID)

Other contributors:

- Leonardo Schwarz <Leonardo.Schwarz@fgcz.ethz.ch> (ORCID) [contributor]

## See Also

Useful links:

- https://github.com/fgcz/rawrr/
- Report bugs at https://github.com/fgcz/rawrr/issues

---

`.benchmark` *Benchmark spectra per second*

---

## Description

Benchmark spectra per second

## Usage

```
.benchmark(rawfile)
```

## Arguments

| | |
|---|---|
| `rawfile` | the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument. |

## Author(s)

Christian Panse 2024-11-05

## Examples

```
sampleFilePath() |> rawrr:::.benchmark() -> S

plot (count / runTimeInSec ~ count,
  log='xy',
  data=S,
  sub = paste0("Overall runtime took ", round(sum(S$runTimeInSec), 3), " seconds."),
  xlab = 'number of random generated scan ids',
  main = "benchmark spectra per second")
```

---

# .downloadNupkgs *Download and install the Thermo Fisher Scientific .NET 8.0 nupkgs*

---

## Description

Download and install the Thermo Fisher Scientific .NET 8.0 nupkgs

## Usage

```
.downloadNupkgs(sourceUrl = .thermofisherlsmsUrl(), force = TRUE)
```

## Arguments

| | |
|---|---|
| sourceUrl | url of nupkgs. |
| force | if TRUE it will overwrite the pkgs. |

## Value

An (invisible) vector of integer code, 0 for success and non-zero for failure. For the "wget" and "curl" methods this is the status code returned by the external program.

## Author(s)

Christian Panse <cp@fgcz.ethz.ch>, 2021, 2024

## .thermofisherlsmsUrl *URL for Thermo Fisher .NET assemblies*

### Description

URL for Thermo Fisher .NET assemblies

### Usage

```
.thermofisherlsmsUrl()
```

### Value

an URL

## auc.rawrrChromatogram *deriving area under the curve (AUC)*

### Description

deriving area under the curve (AUC)

### Usage

```
auc.rawrrChromatogram(x)
```

### Arguments

| | |
|---|---|
| x | an rawrrChromatogram object contains `x$times` and `x$intensities`. `x$times` is assumed to be in minutes. |

### Value

A numeric value.

## basePeak *Base peak of a spectrum*

### Description

Base peak of a spectrum

### Usage

```
basePeak(x)
```

### Arguments

| | |
|---|---|
| x | A rawrrSpectrum object |

### Value

A double vector of length two. The first component is the base peak position (m/z). The second component is the base peak intensity.

### Examples

```
S <- readSpectrum(rawfile = sampleFilePath(), 1)
basePeak(S[[1]])
```

## buildRawrrExe *Build* rawrr.exe *console application.*

### Description

builds `rawrr.exe` file from C# source code requiring .NET SDK. The console application `rawrr.exe` is used by the package's reader functions through a system2 call or a textConnection.

To use this function, ensure that the local RawFileReader NuGet packages are added to the NuGet source list. You can accomplish this by downloading the necessary packages with `rawrr:::.downloadNupkgs()` and subsequently running `rawrr:::.addNupkgSource()`.

### Usage

```
buildRawrrExe()
```

### Value

the return value of the system2 command.

### Author(s)

Christian Panse <cp@fgcz.ethz.ch>, 2021, 2024

## References


- https://www.mono-project.com/docs/advanced/assemblies-and-the-gac/, 2020
- https://planetorbitrap.com/rawfilereader, 2020
- https://github.com/thermofisherlsms/RawFileReader/, 2024
- https://docs.microsoft.com/en-us/dotnet/csharp/language-reference/compiler-options/advanced
- doi:10.1021/acs.jproteome.0c00866


## See Also

installRawrrExe

---

`dependentScan` *Retrieve dependent scan(s) of a scan listed in scan index*

---

## Description

Retrieve dependent scan(s) of a scan listed in scan index

## Usage

```
dependentScan(x, scanNumber)
```

## Arguments

| | |
|---|---|
| `x` | A scan index returned by `readIndex`. |
| `scanNumber` | The scan number that should be inspected for dependent scans. |

## Value

The scan number of the dependent scan(s).

## Examples

```
Idx <- readIndex(rawfile = sampleFilePath())
dependentScan(Idx, scanNumber = 1)
```

## faimsVoltageOn *Is FAIMS Voltage on?*

### Description

Is FAIMS Voltage on?

### Usage

```
faimsVoltageOn(x)
```

### Arguments

| | |
|---|---|
| x | A rawrrSpectrum object |

### Value

A boolean

### Examples

```
S <- readSpectrum(rawfile = sampleFilePath(), 1:10)
try(faimsVoltageOn(S[[1]]))
```

## filter *determine scan numbers which match a specified filter*

### Description

determine scan numbers which match a specified filter

### Usage

```
filter(rawfile, filter = "ms", precision = 10, tmpdir = tempdir())
```

### Arguments

| | |
|---|---|
| rawfile | the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument. |
| filter | scan filter string, e.g., ms or ms2 |
| precision | mass precision, default is 10. |
| tmpdir | defines the directory used to store temporary data generated by the .NET assembly rawrr.exe. The default uses the output of tempdir(). |

### Value

a vecntor of integer values.

## installRawFileReaderDLLs *installRawFileReaderDLLs (deprecated)*

### Description

Download and install the New RawFileReader from Thermo Fisher Scientific .Net assemblies in the directory provided by `rawrrAssemblyPath()`.

### Usage

```
installRawFileReaderDLLs()
```

## installRawrrExe *Download* `rawrr` *assembly*

### Description

downloads and installs the `rawrr.exe` .NET assembly in the directory provided by `rawrrAssemblyPath()`.

### Usage

```
installRawrrExe(
  sourceUrl = "https://fgcz-ms.uzh.ch/~cpanse/rawrr/dotnet/",
  force = FALSE,
  ...
)
```

### Arguments

| | |
|---|---|
| `sourceUrl` | url of `rawrr.exe` assembly. |
| `force` | if `TRUE` it will overwrite the assembly |
| `...` | other parameter for `download.file`. |

### Details

The console application `rawrr` is used by the package's reader functions through a system2 call.

### Value

An integer code, 0 for success and non-zero for failure. For the "wget" and "curl" methods this is the status code returned by the external program.

### See Also

buildRawrrExe

## is.rawrrChromatogram *Function to check if an object is an instance of class* rawrrChromatogram

### Description

Function to check if an object is an instance of class rawrrChromatogram

### Usage

```
is.rawrrChromatogram(x)
```

### Arguments

| | |
|---|---|
| x | x any R object to be tested. |

### Value

TRUE or FALSE

### Author(s)

Tobias Kockmann, 2020.

### Examples

```
rawfile <- sampleFilePath()
C <- readChromatogram(rawfile, mass = 445.1181, tol = 10)
is.rawrrChromatogram(C[[1]])
```

## is.rawrrSpectrum *Function to check if an object is an instance of class* rawrrSpectrum

### Description

Function to check if an object is an instance of class rawrrSpectrum

### Usage

```
is.rawrrSpectrum(x)
```

### Arguments

| | |
|---|---|
| x | any R object to be tested. |

### Value

TRUE or FALSE

### Examples

```
S <- rawrr::sampleFilePath() |> rawrr::readSpectrum(scan = 1:10)
rawrr::is.rawrrSpectrum(S[[1]])
```

---

## is.rawrrSpectrumSet *Function to check if an object is an instance of class rawrrSpectrumSet*

---

### Description

Function to check if an object is an instance of class rawrrSpectrumSet

### Usage

```
is.rawrrSpectrumSet(x)
```

### Arguments

| | |
|---|---|
| x | any R object to be tested. |

### Value

TRUE or FALSE

### Examples

```
rawrr::sampleFilePath() |>
  rawrr::readSpectrum(scan = 1:10) |>
  rawrr::is.rawrrSpectrumSet()
```

---

## makeAccessor *Make accessor function for key value pair returned by RawFileReader*

---

### Description

Make accessor function for key value pair returned by RawFileReader

### Usage

```
makeAccessor(key, returnType = "integer")
```

### Arguments

| | |
|---|---|
| key | An object name found in instance of class rawrrSpectrum |
| returnType | The type used for casting of values |

### Details

This function factory creates accessor functions for class rawrrSpectrum.

### Value

An accessor function

### Author(s)

Tobias Kockmann, 2020

### Examples

```
S <- readSpectrum(rawfile = sampleFilePath(), 1:10)
maxIonTime <- makeAccessor(key = "Max. Ion Time (ms):", returnType = "double")
maxIonTime(S[[1]])
```

---

## massRange *Acquisition/scan range of spectrum*

---

### Description

Acquisition/scan range of spectrum

### Usage

```
massRange(x)
```

### Arguments

| | |
|---|---|
| x | A rawrrSpectrum object |

### Value

A double vector of length two. The first component is the start m/z, the second is the stop m/z value used by the detector during data acquisition. Also referred to as scan range.

### Examples

```
S <- readSpectrum(rawfile = sampleFilePath(), 1)
massRange(S[[1]])
```

## masterScan *Retrieve master scan of scan listed in scan index*

### Description

Retrieve master scan of scan listed in scan index

### Usage

```
masterScan(x, scanNumber)
```

### Arguments

| | |
|---|---|
| x | A scan index returned by readIndex. |
| scanNumber | The scan number that should be inspected for the presence of a master scan. |

### Value

Returns the scan number of the master scan or NA if no master scan exists.

### Examples

```
rawrr::sampleFilePath() |>  rawrr::readIndex() |> rawrr::masterScan(scanNumber = 1)
```

## new_rawrrSpectrum *Create instances of class* rawrrSpectrum

### Description

Developer function.

### Usage

```
new_rawrrSpectrum(
  scan = numeric(),
  massRange = numeric(),
  scanType = character(),
  StartTime = numeric(),
  centroidStream = logical(),
  mZ = numeric(),
  intensity = numeric()
)
```

### Arguments

| | |
|---|---|
| scan | scan number |
| massRange | Mass range covered by spectrum |
| scanType | Character string describing the scan type. |
| StartTime | Retention time in minutes |
| centroidStream | Logical indicating if centroided data is available |
| mZ | m/z values |
| intensity | Intensity values |

### Value

Object of class rawrrSpectrum

### Author(s)

Tobias Kockmann, 2020.

---

## plot.rawrrChromatogram

*Plot* rawrrChromatogram *objects*

---

### Description

Plot rawrrChromatogram objects

### Usage

```
## S3 method for class 'rawrrChromatogram'
plot(x, legend = TRUE, ...)
```

### Arguments

| | |
|---|---|
| x | A rawrrChromatogram object to be plotted. |
| legend | Should legend be printed? |
| ... | Passes additional arguments. |

### Value

This function creates a plot.

### Author(s)

Tobias Kockmann, 2020.

## Examples

```
rawfile <- sampleFilePath()
C <- readChromatogram(rawfile, mass = 445.1181, tol = 10)
plot(C[[1]])
```

---

`plot.rawrrChromatogramSet` *Plot* `rawrrChromatogramSet` *objects*

---

## Description

Plot `rawrrChromatogramSet` objects

## Usage

```
## S3 method for class 'rawrrChromatogramSet'
plot(x, diagnostic = FALSE, ...)
```

## Arguments

| | |
|---|---|
| `x` | A `rawrrChromatogramSet` object to be plotted. |
| `diagnostic` | Show diagnostic legend? |
| `...` | Passes additional arguments. |

## Value

This function creates a plot.

## Author(s)

Tobias Kockmann, 2020.

---

`plot.rawrrSpectrum` *Basic plotting function for instances of* `rawrrSpectrum`

---

## Description

Plot method for objects of class `rawrrSpectrum`.

## Usage

```
## S3 method for class 'rawrrSpectrum'
plot(
  x,
  relative = TRUE,
  centroid = FALSE,
  SN = FALSE,
  legend = TRUE,
  diagnostic = FALSE,
  ...
)
```

## Arguments

| | |
|---|---|
| x | an object of class rawrrSpectrum. |
| relative | If set to TRUE enforces plotting of relative intensities rather than absolute. |
| centroid | Should centroided data be used for plotting? |
| SN | Should Signal/Noise be used for plotting? |
| legend | Should legend be printed? |
| diagnostic | Should this option be applied? The default is FALSE. |
| ... | function passes arbitrary additional arguments. |

## Details

plot.rawrrSpectrum is a low level function that calls base::plot for plotting rawrrSpectrum objects. It passes all additional arguments to plot()

Is usually called by method dispatch.

## Value

This function creates a plot.

## Author(s)

Tobias Kockmann, 2020.

---

# print.rawrrSpectrum *Print method imitate the look and feel of Thermo Fisher Scientific FreeStyle's output*

---

## Description

Print method imitate the look and feel of Thermo Fisher Scientific FreeStyle's output

### Usage

```
## S3 method for class 'rawrrSpectrum'
print(x, ...)
```

### Arguments

| | |
|---|---|
| x | an rawrrSpectrum object. |
| ... | Arguments to be passed to methods. |

### Value

This function creates a print message.

### Author(s)

Christian Panse and Tobias Kockmann, 2020.

---

## rawrrAssemblyPath *Derives the path where all .NET assemblies are stored.*

---

### Description

Derives the path where all .NET assemblies are stored.

### Usage

```
rawrrAssemblyPath()
```

### Value

path

### See Also

installRawrrExe and buildRawrrExe

### Examples

```
rawrrAssemblyPath()
```

## rawrrSpectrum *Create* rawrrSpectrum *objects*

### Description

High-level constructor for instances of class rawrrSpectrum, also named helper function. Currently, mainly to support testing and for demonstration.

### Usage

```
rawrrSpectrum(sim = "TESTPEPTIDE")
```

### Arguments

| | |
|---|---|
| sim | Either example_1 or TESTPEPTIDE |

### Value

Function returns a validated rawrrSpectrum object

### Author(s)

Tobias Kockmann, 2020.

### Examples

```
plot(rawrrSpectrum(sim = "TESTPEPTIDE"))
rawrrSpectrum(sim = "example_1")
```

## readChromatogram *Extracts chromatographic data from a raw file.*

### Description

Extracts chromatographic data from a raw file.

### Usage

```
readChromatogram(
  rawfile,
  mass = NULL,
  tol = 10,
  filter = "ms",
  type = "xic",
  tmpdir = tempdir()
)
```

## Arguments

| | |
|---|---|
| `rawfile` | the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument. |
| `mass` | a vector of mass values iff `type = 'xic'`. |
| `tol` | mass tolerance in ppm iff `type = 'xic'`. |
| `filter` | defines the scan filter, default is `filter="ms"` if a wrong filter is set the function will return `NULL` and draws a warning. |
| `type` | `c(xic, bpc, tic)` for extracted ion , base peak or total ion chromatogram. |
| `tmpdir` | defines the directory used to store temporary data generated by the .NET assembly `rawrr.exe`. The default uses the output of `tempdir()`. |

## Details

Chromatograms come in different flavors but are always signal intensity values as a function of time. Signal intensities can be point estimates from scanning detectors or plain intensities from non-scanning detectors, e.g., UV trace. Scanning detector (mass analyzers) point estimates can be defined in different ways by, for instance, summing all signals of a given spectrum (total ion chromatogram or TIC), or by extracting signal around an expected value (extracted ion chromatogram = XIC), or by using the maximum signal contained in a spectrum (base peak chromatogram = BPC). On top, chromatograms can be computed from pre-filtered lists of scans. A total ion chromatogram (TIC), for instance, is typically generated by iterating over all MS1-level scans.

## Value

chromatogram object(s) containing of a vector of `times` and a corresponding vector of `intensities`.

## Author(s)

Christian Trachsel, Tobias Kockmann and Christian Panse <cp@fgz.ethz.ch> 2018, 2019, 2020.

## References

Automated quality control sample 1 (autoQC01) analyzed across different Thermo Scientific mass spectrometers, MSV000086542.

## See Also

- The Thermo Fisher Scientific RawFileReader C# code snippets https://planetorbitrap.com/rawfilereader.
- https://CRAN.R-project.org/package=protViz
- https://massive.ucsd.edu/ProteoSAFe/dataset.jsp?accession=MSV000086542

## Examples

```
# Example 1: not meaningful but proof-of-concept
(rawfile <- rawrr::sampleFilePath())

rawrr::readChromatogram(rawfile, mass=c(669.8381, 726.8357), tol=1000) |>
    plot()
rawrr::readChromatogram(rawfile, type='bpc') |> plot()
rawrr::readChromatogram(rawfile, type='tic') |> plot()

# Example 2: extract iRT peptides
 if (require(ExperimentHub) & require(protViz)){
iRTpeptide <- c("LGGNEQVTR", "YILAGVENSK", "GTFIIDPGGVIR", "GTFIIDPAAVIR",
  "GAGSSEPVTGLDAK", "TPVISGGPYEYR", "VEATFGVDESNAK",
  "TPVITGAPYEYR", "DGLDAASYYAPVR", "ADVTPADFSEWSK",
  "LFLQFGAQGSPFLK")


# fetch via ExperimentHub
library(ExperimentHub)
eh <- ExperimentHub::ExperimentHub()
EH4547 <- normalizePath(eh[["EH4547"]])

(rawfile <- paste0(EH4547, ".raw"))
if (!file.exists(rawfile)){
    file.link(EH4547, rawfile)
}
op <- par(mfrow=c(2,1))
readChromatogram(rawfile, type='bpc') |> plot()
readChromatogram(rawfile, type='tic') |> plot()
par(op)

# derive [2H+] ions
((protViz::parentIonMass(iRTpeptide) + 1.008) / 2) |>
   readChromatogram(rawfile=rawfile) |>
   plot()
}
```

---

`readFileHeader` *read file header Information*

---

## Description

This function extracts the meta information from a given raw file.

## Usage

```
readFileHeader(rawfile)
```

### Arguments

| | |
|---|---|
| rawfile | the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument. |

### Value

A list object containing the following entries: RAW file version, Creation date, Operator, Number of instruments, Description, Instrument model, Instrument name, Serial number, Software version, Firmware version, Units, Mass resolution, Number of scans, Number of ms2 scans, Scan range, Time range, Mass range, Scan filter (first scan), Scan filter (last scan), Total number of filters, Sample name, Sample id, Sample type, Sample comment, Sample vial, Sample volume, Sample injection volume, Sample row number, Sample dilution factor, or Sample barcode.

### Author(s)

Tobias Kockmann and Christian Panse 2018, 2019, 2020.

### References

Thermo Fisher Scientific's NewRawfileReader C# code snippets https://planetorbitrap.com/rawfilereader.

### Examples

```
rawrr::sampleFilePath() |> readFileHeader()
```

---

## readIndex *Read scan index*

---

### Description

Read scan index

### Usage

```
readIndex(rawfile)
```

### Arguments

| | |
|---|---|
| rawfile | the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument. |

### Value

returns a `data.frame` with the column names scan, scanType, StartTime, precursorMass, MSOrder, charge, masterScan, and dependencyType of all spectra.

## Author(s)

Tobias Kockmann and Christian Panse <cp@fgz.ethz.ch>, 2020, 2021

## Examples

```
Idx <- rawrr::sampleFilePath() |> rawrr::readIndex()
table(Idx$scanType)
plot(Idx$StartTime, Idx$precursorMass, col=as.factor(Idx$charge), pch=16)

table(Idx$MSOrder)
```

---

`readSpectrum` *Reads spectral data from a raw file.*

---

## Description

The function derives spectra of a given raw file and a given vector of scan numbers.

## Usage

```
readSpectrum(
  rawfile,
  scan = NULL,
  tmpdir = tempdir(),
  validate = FALSE,
  mode = ""
)
```

## Arguments

| | |
|---|---|
| `rawfile` | the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument. |
| `scan` | a vector of requested scan numbers. |
| `tmpdir` | defines the directory used to store temporary data generated by the .NET assembly `rawrr.exe`. The default uses the output of `tempdir()`. |
| `validate` | boolean default is `FALSE`. |
| `mode` | if `mode = "barebone"` only mZ (centroidStream.Masses), intensity (centroidStream.Intensities), pepmass, StartTime and charge state is returned. As default mode is `""`. |

## Details

All mass spectra are recorded by scanning detectors (mass analyzers) that log signal intensities for ranges of mass to charge ratios (m/z), also referred to as position. These recordings can be of continuous nature, so-called profile data (p), or appear centroided (c) in case discrete information (tuples of position and intensity values) are sufficient. This heavily compacted data structure is often called a peak list. In addition to signal intensities, a peak list can also cover additional peak attributes like peak resolution (R), charge (z), or local noise estimates. In short, the additional attributes further described the nature of the original profile signal or help to group peak lists with respect to their molecular nature or processing history. A well-known example is the assignment of peaks to peak groups that constitute isotope patterns (M, M+1, M+2, ...). The names of objects encapsulated within `rawrrSpectrum` instances are keys returned by the Thermo Fisher Scientific New RawFileReader API and the corresponding values become data parts of the objects, typically vectors.

## Value

a nested list of `rawrrSpectrum` objects containing more than 50 values of scan information, e.g., the charge state, two vectors containing the mZ and its corresponding intensity values or the AGC information, mass calibration, ion optics ...

## Author(s)

Tobias Kockmann and Christian Panse <cp@fgz.ethz.ch> 2018, 2019, 2020, 2021

## References

- C# code snippets of the NewRawfileReader library https://planetorbitrap.com/rawfilereader.
- rawrr: doi:10.1021/acs.jproteome.0c00866
- Universal Spectrum Explorer: https://www.proteomicsdb.org/use/ doi:10.1021/acs.jproteome.1c00096

## See Also

https://massive.ucsd.edu/ProteoSAFe/dataset.jsp?accession=MSV000086542

## Examples

```
# Example 1
S <- rawrr::sampleFilePath() |> rawrr::readSpectrum(scan = 1:9)

S[[1]]

names(S[[1]])

plot(S[[1]])



# Example 2 - find best peptide spectrum match using the |> pipe operator
# fetch via ExperimentHub
```

```
if (require(ExperimentHub) & require(protViz)){
eh <- ExperimentHub::ExperimentHub()
EH4547 <- normalizePath(eh[["EH4547"]])

(rawfile <- paste0(EH4547, ".raw"))
if (!file.exists(rawfile)){
    file.link(EH4547, rawfile)
}

GAG <- "GAGSSEPVTGLDAK"

.bestPeptideSpectrumMatch <- function(rawfile,
    sequence="GAGSSEPVTGLDAK"){
    readIndex(rawfile) |>
        subset(abs((1.008 + (protViz::parentIonMass(sequence) - 1.008) / 2) -
            precursorMass) < 0.001, select = scan) |>
        unlist() |>
        readSpectrum(rawfile = rawfile) |>
        lapply(function(x) {
          y <- protViz::psm(sequence = GAG, spec=x, plot=FALSE);
          y$scan <- x$scan; y
        }) |>
        lapply(FUN= function(x){
          score <- sum(abs(x$mZ.Da.error) < 0.01);
          cbind(scan=x$scan, score=score)
        }) |>
        (function(x) as.data.frame(Reduce(rbind, x)))() |>
        subset(score > 0) |>
        (function(x) x[order(x$score, decreasing = TRUE),
            'scan'])() |>
        head(1)
}

start_time <- Sys.time()
bestMatch <- .bestPeptideSpectrumMatch(rawfile, GAG) |>
    rawrr::readSpectrum(rawfile=rawfile) |>
    lapply(function(x) protViz::peakplot(peptideSequence = GAG, x))

end_time <- Sys.time()
end_time - start_time

# Example 3
# using proteomicsdb \doi{10.1101/2020.09.08.287557}
# through https://www.proteomicsdb.org/use/

.UniversalSpectrumExplorer <- function(x, sequence){
    m <- protViz::psm( sequence, x)
    cat(paste(x$mZ[m$idx], "\t", x$intensity[m$idx]), sep = "\n")
}

rawrr::readSpectrum(rawfile=rawfile, 11091) |>
   lapply(function(x).UniversalSpectrumExplorer(x, sequence = GAG))
 }
```

## readTrailer *Read and extract scan trailer from TFS raw files.*

### Description

Read and extract scan trailer from TFS raw files.

### Usage

```
readTrailer(rawfile, label = NULL)
```

### Arguments

| | |
|---|---|
| rawfile | the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument. |
| label | if NULL; the function scans for all available labels. |

### Value

an vector of trailers or values of a given trailer. Of note, the values are usually returned as a character.

### Examples

```
rawrr::sampleFilePath() |> rawrr:::readTrailer()
rawrr::sampleFilePath() |> rawrr:::readTrailer("AGC:") |> head()
```

## sampleFilePath *A small file size* sample.raw *BLOB*

### Description

The binary example file sample.raw, shipped with the package, contains 574 Fourier-transformed Orbitrap spectra (FTMS) recorded on a Thermo Fisher Scientific Q Exactive HF-X. The mass spectrometer was operated in line with a nano electrospray source (NSI) in positive mode (+). All spectra were written to disk after applying centroiding (c) and lock mass correction.

### Usage

```
sampleFilePath()
```

### Details

Thermo Fisher Scientific Q Exactive HF-X raw file of size 1.5M bytes and checksum MD5 (sample.raw) = fe67058456c79af7442316c474d20e96. Additional raw data for demonstration and extended testing is available through MSV000086542 and the tartare package. **Lions love raw meat!**

## Value

file path of the sample.raw location.

## Author(s)

Tobias Kockmann, 2018, 2019.

## References

- Bioconductor tartare package.
- Automated quality control sample 1 (autoQC01) analyzed across different Thermo Fisher Scientific mass spectrometers, MSV000086542.

## Examples

```
sampleFilePath()
```

---

# scanNumber *Accessor function for scan number of* rawrrSpectrum *objects*

---

## Description

Accessor function for scan number of rawrrSpectrum objects

## Usage

```
scanNumber(x)
```

## Arguments

| | |
|---|---|
| x | A rawrrSpectrum object |

## Details

This accessor function returns the scan number of a mass spectrum stored as rawrrSpectrum object. Scan numbers are equal to the scan index $j$ running from 1 to $n$ with $n$ being the last scan of a raw file.

## Value

The scan number of type integer

## Examples

```
S <- readSpectrum(rawfile = sampleFilePath(), 1:10)
scanNumber(S[[1]])
```

## summary.rawrrChromatogram *Text summary of chromatogram*

### Description

Text summary of chromatogram

### Usage

```
## S3 method for class 'rawrrChromatogram'
summary(object, ...)
```

### Arguments

| | |
|---|---|
| object | A rawrrChromatogram object |
| ... | Function passes additional arguments. |

### Value

A rawrrChromatogram object

### Examples

```
C <- readChromatogram(rawfile = sampleFilePath(),
mass = c(445.1181, 519.1367))
summary(C[[1]])
summary(C[[2]])
```

## summary.rawrrSpectrum *Basic summary function*

### Description

Basic summary function

### Usage

```
## S3 method for class 'rawrrSpectrum'
summary(object, ...)
```

### Arguments

| | |
|---|---|
| object | an rawrrSpectrum object. |
| ... | Arguments to be passed to methods. |

## Value

This function creates a print message.

## Author(s)

Christian Panse and Tobias Kockmann, 2020.

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`tic` *Total ion current of a spectrum*

---

## Description

Total ion current of a spectrum

## Usage

```
tic(x)
```

## Arguments

| | |
|---|---|
| `x` | A rawrrSpectrum object |

## Value

A double vector of length one.

## Examples

```
S <- readSpectrum(rawfile = sampleFilePath(), 1)
tic(S[[1]])
```

---

`validate_rawrrIndex` *Validate output of the readIndex function*

---

## Description

Checks the validity of an `readIndex` returned object.

## Usage

```
validate_rawrrIndex(x)
```

## Arguments

| | |
|---|---|
| `x` | object to be validated. |

### Value

Validated `data.frame` of `readIndex` object

### Author(s)

Tobias Kockmann and Christian Panse, 2020-12-09.

### Examples

```
rawrr::sampleFilePath() |> rawrr::readIndex() |> rawrr::validate_rawrrIndex()
```

---

## validate_rawrrSpectrum

*Validate instance of class rawrrSpectrum*

---

### Description

Checks the validity of `rawrrSpectrum` object attributes.

### Usage

```
validate_rawrrSpectrum(x)
```

### Arguments

| | |
|---|---|
| `x` | object to be validated. |

### Value

Validated `rawrrSpectrum` object

### Author(s)

Tobias Kockmann and Christian Panse, 2020.

### Examples

```
S <- rawrr::sampleFilePath() |>
  rawrr::readSpectrum(scan = 1:9, validate=TRUE)
```

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