Package: SpectraVis (via r-universe)

August 22, 2024

Title Visualising and Exploring Spectra Data

Version 0.3.0

Description This package defines a set of helper function to visualise and explore mass spectrometry data stored as Spectra objects.

Depends Spectra

Imports PSMatch, shiny, plotly, MsCoreUtils

Suggests msdata, testthat

Remotes RforMassSpectrometry/PSMatch

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RemoteRef HEAD

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Contents

browseSpectra *Browse spectra in a Spectra object*

Description

The `browseSpectra()` function opens a simple shiny application that allows to browse trough the individual scans of a `Spectra` object. The title of the scans contains the MS level, the retention time, if available the precursor m/z and precursor charge and a peptides sequence (as defined in the `sequence` spectra variable) and the index of the scan. If a scans has a sequence (as defined in the `sequence` spectra variable), the matching fragments (as defined by `PSMatch::calculateFragments()` are labelled, otherwise the most intense peaks (as defined as those that have an intensity as high as half the highest peak) are labelled with their m/z.

See `?SpectraVis` for an example.

Usage

```
browseSpectra(object)
```

Arguments

`object`	A non-empty instance of class `Spectra`.

Value

An object that represents the app.

Author(s)

Laurent Gatto

plotlySpectra *Interactive visualisation of a single spectrum*

Description

The `plotlySpectra()` function displays a single spectrum stored in a `Spectra` object using the `plotly::plot_ly()` function.

See `?SpectraVis` for an example.

Usage

```
plotlySpectra(object)
```

Arguments

`object`	A instance of class `Spectra` of length 1.

Value

A `plotly` object.

Author(s)

Laurent Gatto, Johannes Rainer

Examples

```
library(msdata)
fl <- system.file("TripleTOF-SWATH", "PestMix1_DDA.mzML", package = "msdata")
pest_ms2 <- filterMsLevel(Spectra(fl), 2L)

plotlySpectra(pest_ms2[950])
```

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plotlySpectraMirror *Interactive visualisation of a mirror plot*

Description

The `plotlySpectraMirror` function creates an interactive *mirror plot* comparing two spectra `x` and `y` with each other. Peaks with matching m/z values (considering `ppm` and `tolerance`) are indicated with a point which size can be specified with parameter `matchSize`.

See also `plotSpectraMirror()` for a non-interactive version of this plot.

Usage

```
plotlySpectraMirror(
  x,
  y,
  xLabel = "",
  xColor = "#737373",
  yLabel = "",
  yColor = "#737373",
  matchSize = 5,
  ppm = 20,
  tolerance = 0
)
```

Arguments

`x`	A `Spectra()` object of length 1.
`y`	A `Spectra()` object of length 1.
`xLabel`	Optional `character(1)` with the label (name) of `x`.
`xColor`	Color for peaks of spectrum `x`.
`yLabel`	Optional `character(1)` with the label (name) of `y`.

yColor	Color for peaks of spectrum y.
matchSize	numeric(1) defining the size of the point that will be used to indicate peaks in x and y with matching m/z.
ppm	numeric(1) with the m/z relative acceptable difference (in ppm) for peaks to be considered matching (see common() for more details).
tolerance	numeric(1) with the absolute acceptable difference of m/z values for peaks to be considered matching (see common() for more details).

Value

A plotly object

Author(s)

Johannes Rainer

Examples

```
## Load example data.
library(msdata)
fl <- system.file("TripleTOF-SWATH", "PestMix1_DDA.mzML", package = "msdata")
pest_ms2 <- filterMsLevel(Spectra(fl), 2L)

plotlySpectraMirror(pest_ms2[948], pest_ms2[950])

plotlySpectraMirror(pest_ms2[948], pest_ms2[959], xLabel = "query",
    yLabel = "target", xColor = "red", yColor = "blue")
```

SpectraVis *SpectraVis: Visualising and Exploring Spectra Data*

Description

This package defines a set of helper function to visualise and explore mass spectrometry data stored as Spectra objects.

SpectraVis functions

- plotlySpectra: Interactive visualisation of a single spectrum.
- browseSpectra: Browse spectra in a Spectra object.

Examples

```
f <- msdata::proteomics(pattern = "MS3TMT10", full.names = TRUE)
sp <- Spectra(f)
sp

if (interactive())
   browseSpectra(sp)

## Use Ctrl+C to interrupt R and stop the application

if (interactive())
   plotlySpectra(sp[1])
```

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