Package 'IsoCor'

September 10, 2024

Title Analyze Isotope Ratios in a 'Shiny'-App

Version 0.2.8

Date 2024-09-09

Description Analyzing Inductively Coupled Plasma - Mass Spectrometry (ICP-MS) measurement data to evaluate isotope ratios (IRs) is a complex process. The 'IsoCor' package facilitates this process and renders it reproducible by providing a function to run a 'Shiny'-App locally in any web browser. In this App the user can upload data files of various formats, select ion traces, apply peak detection and perform calculation of IRs and delta values. Results are provided as figures and tables and can be exported. The App, therefore, facilitates data processing of ICP-MS experiments to quickly obtain optimal processing parameters compared to traditional 'Excel' worksheet based approaches. A more detailed description can be found in the corresponding article <doi:10.1039/D2JA00208F>. The most recent version of 'IsoCor' can be tested online at <https://apps.bam.de/shn00/IsoCor/>.

License GPL (>= 3)

URL https://github.com/janlisec/IsoCor

Depends R (>= 4.1.0)

Imports bslib, config, DT, golem, MALDIquant, markdown (>= 1.5.0), plyr, shiny, shinyalert (>= 3.1), shinyjs

Suggests shinytest2, testthat (>= 3.0.0), vdiffr

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LazyDataCompression bzip2

RoxygenNote 7.3.2

NeedsCompilation no

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Contents

`find_peak_boundaries` *find_peak_boundaries*

Description

`find_peak_boundaries` will find the start and end point of a peak based on curve derivative.

Usage

```
find_peak_boundaries(
  int = NULL,
  p = which.max(int),
  k = 3,
  min_scans = 3,
  noise = 0
)
```

Arguments

`int`	Numeric vector (of intensity values).
`p`	Index of peak position (usually 'which.max(int)).
`k`	Number of scans at peak boarder to confirm peak valley.
`min_scans`	Minimum number of scans in front or tail.
`noise`	A threshold value. All Values below or equal to noise will be set to zero.

Details

This function provides a simple detection algorithm for peak boundaries. It will accept a numeric vector as input and determine relative to the global maximum (or a user provided local maximum) the left and right border where intensity decrease ends and intensity is increasing again.

Value

A numeric vector of length 2 giving the indexes of peak start and peak end.

Examples

```
## Not run:
x <- sin(seq(-pi,2*pi,0.01))+1
plot(x)
abline(v=find_peak_boundaries(x))

## End(Not run)
```

`ic_app` *ic_app.*

Description

`ic_app` will start a shiny app that allows to upload raw data, process selectively and analyze different methods of ratio calculation between two intensity traces.

Usage

```
ic_app(...)
```

Arguments

`...`	Options passed to golem::with_golem_options.

Details

The app is described in detail in doi:10.1039/D2JA00208F.

Value

A shiny app object. This will effectively launch a browser and start the app on local port 7462.

See Also

iso_ratio

isotopes *isotopes.*

Description

isotopes.

Usage

```
data(isotopes)
```

Format

A data.frame of chemical isotopes providing mass and natural abundance.

Source

R-package enviPat

iso_ratio *iso_ratio*

Description

`iso_ratio` will calculate a robust estimate of an isotopic ratio between intensity values of 2 mass traces.

Usage

```
iso_ratio(data, method = c("PBP", "PAI", "LRS"), thr = 1)
```

Arguments

`data`	data.frame with two columns specifying data for isotope 1 and 2 respectively.
`method`	Method to calculate the isotope ratio.
`thr`	Threshold between 0..1 to limit the peaks scans used in the calculation (1=all scans, 0=apex only).

Details

Within `ic_app` we compute estimates for isotope ratios using raw data and several processing steps. `iso_ratio` is internally used to perform this calculation and could be used in an external data processing pipeline without the app context. However, users would need to extract intensity vectors of isotope peaks from raw data independently. **Note!** All non-finite values and x==0 will be removed before calculation.

Value

A single numeric value. The robust ratio estimate calculated from `data`.

Examples

```
peak1 <- 1 + cos(x = seq(-pi, pi, length.out = 100))
peak2 <- 0.05 * peak1 * runif(n = 100, min = 1, max = 1.01)
iso_ratio(data = cbind(peak1, peak2))
```

`mass_bias` *mass_bias.*

Description

`mass_bias` will calculate a correction factor K to scale isotopic ratios and thereby account for machine variance.

Usage

```
mass_bias(
  mi_amu = 0,
  si_amu = 0,
  method = c("Linear", "Russel", "Exponential"),
  f_value = 0
)
```

Arguments

`mi_amu`	atomic mass of MI isotope.
`si_amu`	atomic mass of SI isotope
`method`	Method to calculate the mass bias.
`f_value`	f_value to be used within the method calculation.

Details

Currently, 3 methods are available to calculate the mass bias, Linear, Russel and Exponential. They all depend on the atomic mass of the two ion traces and a f-value which can be provided as parameters to the function.

Value

A single numeric value K to be used for scaling.

Examples

```
IsoCor::mass_bias(32, 34, "Linear", 0.1)
```

read_raw_data *read_raw_data*

Description

read_raw_data will import ICP MS data in various file formats.

Usage

```
read_raw_data(path, format = c("exp", "icp", "data", "generic"))
```

Arguments

path	Valid file path.
format	Character specifying the import file format.

Details

Try to specify 'format' parameter to find a method suitable for your files or select 'generic' which will import a tab delimited file with 3 columns defining RT, MI and SI respectively. You may check why data import of your files fails in the app on this function and potentially extend it to handle your files.

Value

A data.frame.

Examples

```
str(IsoCor::read_raw_data(path = ""))
```

testdata *testdata.*

Description

testdata.

Usage

```
data(testdata)
```

Format

A list of 3 exp spectra files converted by read_raw_data.

Source

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`testdata_IDMS` *testdata_IDMS.*

Description

testdata_IDMS.

Usage

```
data(testdata_IDMS)
```

Format

A list of 3 txt spectra files converted by read_raw_data.

Source

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