

Package ‘IsoCor’

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Title Analyze Isotope Ratios in a 'Shiny'-App

Version 0.1.40

Date 2022-09-06

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 "Data processing made easy: standalone tool for automated calculation of isotope ratio from transient signals – IsoCor" by Tukhmetova et al. in Journal of Analytical Atomic Spectrometry (JAAS). The most recent version of 'IsoCor' can be tested online at <https://jali.shinyapps.io/isocor>.

URL <https://jali.shinyapps.io/isocor>

License GPL (>= 3)

Encoding UTF-8

RoxygenNote 7.2.1

Depends R (>= 3.50)

Imports bsplus, DT, golem, htmltools, MALDIquant, markdown, plyr, rmarkdown, shiny, shinyalert, shinyjs

Suggests config, pkgload, rsconnect, testthat (>= 3.0.0)

NeedsCompilation no

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ic_app	<i>ic_app</i>
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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()
```

Details

The app is described in detail in [this publication](#).

Value

A shiny app object.

References

<https://jali.shinyapps.io/IsoCor>

See Also

[iso_ratio](#)

isotopes	<i>isotopes.</i>
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Description

isotopes.

Usage

```
data(isotopes)
```

Format

A data.frame of chemical isotopes.

Source

R-package enviPat

iso_ratio	<i>iso_ratio</i>
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Description

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

Usage

```
iso_ratio(  
  data = data.frame(X = rnorm(10), Y = rnorm(10)),  
  method = c("PBP", "PAI", "LRS")[1],  
  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	<i>mass_bias.</i>
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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", "Russet", "Exponential")[1],
  f_value = 0
)
```

Arguments

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

Details

tbd.

Value

A single numeric value K to be used for scaling.

Examples

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

read_raw_data	<i>read_raw_data</i>
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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 filepath.
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.

Value

A data.frame.

Examples

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

testdata	<i>testdata.</i>
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Description

testdata.

Usage

```
data(testdata)
```

Format

A list of 3 exp spectra files converted by read_raw_data.

Source

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