Package 'IsoCorrectoR'

October 16, 2019

Title Correction for natural isotope abundance and tracer purity in MS
and MS/MS data from stable isotope labeling experiments

Version 1.2.1

Imports dplyr, magrittr, methods, quadprog, readr, readxl, stringr,
tibble, tools, utils, pracma, WriteXLS

Description IsoCorrectoR performs the correction of mass spectrometry data from stable isotope la-
beling/tracing metabolomics experiments with regard to natural isotope abundance and tracer im-
purity. Data from both MS and MS/MS measurements can be corrected (with any tracer iso-
tope: 13C, 15N, 18O...), as well as high resolution MS data from multiple-tracer experi-
ments (e.g. 13C and 15N used simultaneously). See the Bioconductor package IsoCorrec-
toRGUI for a graphical user interface to IsoCorrectoR.

Depends R (>= 3.5)

URL https://genomics.ur.de/files/IsoCorrectoR/

License GPL-3

LazyData TRUE

NeedsCompilation no

biocViews Software, Metabolomics, MassSpectrometry, Preprocessing,
ImmunoOncology

RoxygenNote 6.1.1

Suggests IsoCorrectoRGUI, knitr, rmarkdown, testthat

VignetteBuilder knitr

git_url https://git.bioconductor.org/packages/IsoCorrectoR

git_branch RELEASE_3_9

git_last_commit 3e7a164

git_last_commit_date 2019-05-22

Date/Publication 2019-10-15

Author Christian Kohler [cre, aut],
Paul Heinrich [aut]

Maintainer Christian Kohler <christian.kohler@ur.de>

R topics documented:

1

IsoCorrection	*Algorithm For Natural Isotope Abundance And Tracer Purity Correction Of Data From Stable Isotope Labeling Experiments*

Description

IsoCorrection is the main function of the IsoCorrectoR package. It performs the correction of mass spectrometry data from stable isotope labeling experiments with regard to natural abundance and tracer purity. Data from both MS and MS/MS experiments can be corrected (with any tracer isotope: 13C, 15N, 18O...), as well as high resolution data from multiple-tracer experiments (e.g. 13C and 15N used simultaneously).

Usage

```
IsoCorrection(MeasurementFile = NA, ElementFile = NA,
  MoleculeFile = NA, CorrectTracerImpurity = FALSE,
  CorrectTracerElementCore = TRUE, CalculateMeanEnrichment = TRUE,
  UltraHighRes = FALSE, DirOut = ".", FileOut = "result",
  FileOutFormat = "csv", ReturnResultsObject = TRUE,
  CorrectAlsoMonoisotopic = FALSE, CalculationThreshold = 10^-8,
  CalculationThreshold_UHR = 8, verbose = FALSE, Testmode = FALSE)
```

Arguments

MeasurementFile

        Required. The file that contains the measured data to be corrected. Only ".xls",".xlsx" and ".csv" file formats are supported.

ElementFile   Required. The file that contains the element information required for correction. Only ".xls",".xlsx" and ".csv" file formats are supported.

MoleculeFile   Required. The file that contains the information on the molecules for which data is to be corrected. Only ".xls",".xlsx" and ".csv" file formats are supported.

CorrectTracerImpurity

        Logical. If TRUE, correction for isotopic impurity of the tracer substrate is performed.

CorrectTracerElementCore

        Logical. If TRUE (recommended!), the tracer element atoms in the core module (usually the part of the molecule that does not come from derivatization) are considered when correcting.

CalculateMeanEnrichment

        Logical. If TRUE, the mean isotopic enrichment is calculated for each molecule.

UltraHighRes   Logical. If TRUE, high resolution correction is performed on the data. Should only be set to TRUE, if you know that you have high resolution data.

DirOut   Character String. Defines the directory the corrected data and log-file should be written to. Default directory is set to current working directoy ('.').

FileOut   Character String. Defines the name of the file that contains the corrected data. The name of the fill will be IsoCorrectoR_<FileOut>.<FileFormat>. If the format is set to "csv", the name will also contain the type of the corrected data in the respective file.

FileOutFormat   Character String. Defines the format of the files that contain the corrected data. Can either be "csv" or "xls". If set to "csv", multiple files will be generated, one for each type of corrected data (eg. corrected data, fractions, mean enrichment...). If set to "xls", all correction results are provided in one excel file in different sheets.

ReturnResultsObject

Logical. If TRUE, the correction results are returned as a list in the current R_session in addition to writing the results to a file. This is useful if the corrected data has to be further processed directly in R.

CorrectAlsoMonoisotopic

Logical. If TRUE, monoisotopic correction results are also provided.

CalculationThreshold

(Advanced Option) Numeric. Defines a threshold to stop probability calculations at for making correction faster (normal resolution mode). Should be left at the default value.

CalculationThreshold_UHR

(Advanced Option) Numeric. Defines a threshold to stop probability calculations at for making correction faster (high resolution mode). Should be left at the default value.

verbose   Logical. If TRUE, status messages are sent to standard output.

Testmode   Logical. If TRUE, starts a testmode for development purposes. Not required for users of IsoCorrectoR.

Value

The function returns a list with 4 elements

success: string that is "TRUE" if the correction was successful, "FALSE" if an error occured and "WARNINGS" if warnings occured

results: a list containing a dataframe for each type of corrected data (normal, fractions, mean enrichment ...). Will be NA if ReturnResultsObject is set to FALSE

log: list containing log information on the correction run (parameters, file names and paths, warnings and errors)

error: contains a string with the associated error message if an error occurred, empty otherwise

References

See Reference 1 LinktoIsoCorrectoR-Paper

Examples

```
# Normal resolution data

  # 1) get path of example files
  path.molecule <- system.file("extdata","normal_resolution","MoleculeFile.csv",
    package = "IsoCorrectoR", mustWork = TRUE);
  path.element <- system.file("extdata","normal_resolution","ElementFile.csv",
    package = "IsoCorrectoR", mustWork = TRUE);
  path.measurement <- system.file("extdata","normal_resolution","MeasurementFile.csv",
    package = "IsoCorrectoR", mustWork = TRUE);
```

```
    # 2) run correction algorithm and save results in variable
    correctionResults <- IsoCorrection(MeasurementFile=path.measurement,
       ElementFile=path.element,
      MoleculeFile=path.molecule)

  # High resolution data

    # 1) get path of example files
    path.molecule <- system.file("extdata","high_resolution","MoleculeFile.csv",
       package = "IsoCorrectoR", mustWork = TRUE);
    path.element <- system.file("extdata","high_resolution","ElementFile.csv",
       package = "IsoCorrectoR", mustWork = TRUE);
    path.measurement <- system.file("extdata","high_resolution","MeasurementFile.csv",
       package = "IsoCorrectoR", mustWork = TRUE);

    # 2) run correction algorithm and save results in variable
    correctionResults <- IsoCorrection(MeasurementFile=path.measurement,
       ElementFile=path.element,
      MoleculeFile=path.molecule,UltraHighRes=TRUE)
```

IsoCorrectoR   *IsoCorrectoR example data*

Description

Example data for the IsoCorrectoR package

Usage

```
data(IsoCorrectoR)
```

Format

A list with four elements, namely

tool_features: overview of correction features as provided by various tools IsoCorrectoR is compared with.

element_file: example data for an Element file. This information is independent of the resolution type (normal or high)

normal_resolution: list with two elements, containing examples for normal resolution data: molecule information and measurement data

high_resolution: list with two elements, containing examples for high resolution data: molecule information and measurement data

Author(s)

Paul Heinrich, Christian Kohler

Index