# Package 'IsoCorrectoR'

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

**Version** 1.29.0

**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 labeling/tracing metabolomics experiments with regard to natural isotope abundance and tracer impurity. Data from both MS and MS/MS measurements can be corrected (with any tracer isotope: 13C, 15N, 18O...), as well as ultra-high resolution MS data from multiple-tracer experiments (e.g. 13C and 15N used simultaneously). See the Bioconductor package IsoCorrectoRGUI for a graphical user interface to IsoCorrectoR. NOTE: With R version 4.0.0, writing correction results to Excel files may currently not work on Windows. However, writing results to csv works as before.

**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, BiocStyle

**VignetteBuilder** knitr

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

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

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## 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)
```

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`IsoCorrectoR` *IsoCorrectoR example data*

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## 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)

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