

Package ‘accucor’

May 7, 2026

Type Package

Title Natural Abundance Correction of Mass Spectrometer Data

Version 0.3.1

Description An isotope natural abundance correction algorithm that is needed especially for high resolution mass spectrometers. Supports correction for 13C, 2H and 15N. Su X, Lu W and Rabinowitz J (2017) <[doi:10.1021/acs.analchem.7b00396](https://doi.org/10.1021/acs.analchem.7b00396)>.

URL <https://github.com/XiaoyangSu/AccuCor>

BugReports <https://github.com/XiaoyangSu/AccuCor/issues>

License MIT + file LICENSE

Encoding UTF-8

Imports nnl, dplyr, stringr, readxl, readr, rlang, tibble, writexl, CHNOSZ

RoxygenNote 7.2.3

Suggests testthat

NeedsCompilation no

Author Xiaoyang Su [aut] (ORCID: <<https://orcid.org/0000-0001-8081-1396>>),
Lance Parsons [aut, cre] (ORCID:
<<https://orcid.org/0000-0002-8521-714X>>),
Yujue Wang [ctb] (ORCID: <<https://orcid.org/0000-0001-7088-1729>>),
Princeton University [cph]

Maintainer Lance Parsons <lparsons@princeton.edu>

Repository CRAN

Date/Publication 2023-09-14 15:30:05 UTC

Contents

| | |
|---------------------------|---|
| accucor | 2 |
| carbon_isotope_correction | 3 |
| clean_data_frame | 4 |

| | |
|--|----------|
| deuterium_isotope_correction | 4 |
| natural_abundance_correction | 5 |
| nitrogen_isotope_correction | 7 |
| read_elmaven | 8 |
| Index | 9 |

| | |
|---------|--|
| accucor | <i>accucor: A package for natural abundance correction of mass spectrometer data</i> |
|---------|--|

Description

AccuCor is an isotope natural abundance correction algorithm that is needed especially for high resolution mass spectrometers. AccuCor supports correction for ^{13}C , ^2H and ^{15}N .

AccuCor functions

[natural_abundance_correction](#)

Author(s)

Maintainer: Lance Parsons <lparsons@princeton.edu> ([ORCID](#))

Authors:

- Xiaoyang Su <xs137@rwjms.rutgers.edu> ([ORCID](#))

Other contributors:

- Yujue Wang <yw429@rwjms.rutgers.edu> ([ORCID](#)) [contributor]
- Princeton University [copyright holder]

See Also

Useful links:

- <https://github.com/XiaoyangSu/AccuCor>
- Report bugs at <https://github.com/XiaoyangSu/AccuCor/issues>

`carbon_isotope_correction`*Natural Abundance carbon isotope correction for one metabolite*

Description

Natural Abundance carbon isotope correction for one metabolite

Usage

```
carbon_isotope_correction(  
  formula,  
  datamatrix,  
  label,  
  Resolution,  
  ResDefAt = 200,  
  purity = 0.99,  
  ReportPoolSize = TRUE  
)
```

Arguments

| | |
|-----------------------------|---|
| <code>formula</code> | String representing molecular formula |
| <code>datamatrix</code> | Matrix of abundances for each sample for each isotope |
| <code>label</code> | vector of integer labels |
| <code>Resolution</code> | For Exactive, the Resolution is 100000, defined at Mw 200 |
| <code>ResDefAt</code> | Resolution defined at (in Mw), e.g. 200 Mw |
| <code>purity</code> | Carbon 13 purity, default: 0.99 |
| <code>ReportPoolSize</code> | default: TRUE |

Value

Named list of matrices: 'Corrected', 'Normalized', 'PoolBeforeDF', and 'PoolAfterDF'.

Examples

```
## Not run:  
carbon_isotope_correction(  
  formula = "C6H13O9P",  
  datamatrix = DataMatrix,  
  label = c(0, 1, 2, 3, 4, 5),  
  Resolution = 100000  
)  
  
## End(Not run)
```

| | |
|------------------|--|
| clean_data_frame | <i>Standardize data frame columns and data types</i> |
|------------------|--|

Description

Standardize data frame columns and data types

Usage

```
clean_data_frame(df, columns_to_skip = NULL)
```

Arguments

| | |
|-----------------|---|
| df | Data frame to clean |
| columns_to_skip | Specify column heading to skip. All other columns not named 'compound', 'formula', and 'isotopelabel' will be assumed to be sample names. |

Value

"cleaned" data.frame which with columns 'compound', 'formula', 'isotope_label', 'label_index', followed by columns for each sample

| | |
|------------------------------|--|
| deuterium_isotope_correction | <i>Natural Abundance deuterium isotope correction for one metabolite</i> |
|------------------------------|--|

Description

Natural Abundance deuterium isotope correction for one metabolite

Usage

```
deuterium_isotope_correction(  
  formula,  
  datamatrix,  
  label,  
  Resolution,  
  ResDefAt = 200,  
  purity = 0.99,  
  ReportPoolSize = TRUE  
)
```

Arguments

| | |
|----------------|---|
| formula | String representing molecular formula |
| datamatrix | Matrix of abundances for each sample for each isotope |
| label | vector of integer labels |
| Resolution | For Exactive, the Resolution is 100000, defined at Mw 200 |
| ResDefAt | Resolution defined at (in Mw), e.g. 200 Mw |
| purity | Deuterium purity, default: 0.99 |
| ReportPoolSize | default: TRUE |

Value

Named list of matrices: 'Corrected', 'Normalized', 'PoolBeforeDF', and 'PoolAfterDF'.

Examples

```
## Not run:
deuterium_isotope_correction(
  formula = "C6H13O9P",
  datamatrix = DataMatrix,
  label = c(0, 1),
  Resolution = 100000
)

## End(Not run)
```

natural_abundance_correction

Natural Abundance correction for mass spectrometry data

Description

natural_abundance_correction returns the corrected and normalized intensities of isotopically labeled mass spectrometry data. It was designed to work with input data from **EI-MAVEN** and **MAVEN** software.

Usage

```
natural_abundance_correction(
  data,
  sheet = NULL,
  compound_database = NULL,
  output_base = NULL,
  output_filetype = "xlsx",
  columns_to_skip = NULL,
  resolution,
  resolution_defined_at = 200,
```

```

    purity = NULL,
    report_pool_size_before_df = FALSE,
    path = NULL
)

```

Arguments

| | |
|----------------------------|---|
| data | Path to input data file (xlsx, xls, csv, txt, or tsv) OR dataframe. If dataframe is specified, specify output_base to output files automatically written. |
| sheet | Name of sheet in xlsx file with columns 'compound', 'formula', 'isotopelabel', and one column per sample. Defaults to the first sheet. |
| compound_database | Path to compound database in csv format. Only used for classic MAVEN style input when formula is not specified. |
| output_base | Path to basename of output file, default is the basename of the input path. '_corrected' will be appended. If 'FALSE' then no output file is written. |
| output_filetype | Filetype of the output file, one of: 'xls', 'xlsx', 'csv', or 'tsv'. The default is 'xlsx'. |
| columns_to_skip | Specify column heading to skip. All other columns not named 'compound', 'formula', and 'isotopelabel' will be assumed to be sample names. |
| resolution | For Exactive, the resolution is 100000, defined at Mw 200 |
| resolution_defined_at | Mw at which the resolution is defined, default 200 Mw |
| purity | Isotope purity, default: Carbon 0.99; Deuterium 0.98; Nitrogen 0.99 |
| report_pool_size_before_df | Report PoolSizeBeforeDF, default = FALSE |
| path | Deprecated. Specify path to input data file (alias for 'data'). |

Details

C13, H2, and N15 isotopes are supported. The isotopes are detected from the isotopeLabel column of the input file. The expected label text is C13-label-#. D-label-#. or N15-label-#. Parent (unlabeled) compounds are specified by C12 PARENT.

Value

Named list of matrices: 'Corrected', 'Normalized', 'PoolBeforeDF', and 'PoolAfterDF'.

Examples

```

## Not run:
natural_abundance_correction("inst/extdata/C_Sample_Input_Simple.xlsx",
  Resolution = 100000, ResDefAt = 200
)

## End(Not run)

```

`nitrogen_isotope_correction`*Natural Abundance deuterium isotope correction for one metabolite*

Description

Natural Abundance deuterium isotope correction for one metabolite

Usage

```
nitrogen_isotope_correction(  
  formula,  
  datamatrix,  
  label,  
  Resolution,  
  ResDefAt = 200,  
  purity = 0.99,  
  ReportPoolSize = TRUE  
)
```

Arguments

| | |
|-----------------------------|---|
| <code>formula</code> | String representing molecular formula |
| <code>datamatrix</code> | Matrix of abundances for each sample for each isotope |
| <code>label</code> | vector of integer labels |
| <code>Resolution</code> | For Exactive, the Resolution is 100000, defined at Mw 200 |
| <code>ResDefAt</code> | Resolution defined at (in Mw), e.g. 200 Mw |
| <code>purity</code> | Nitrogen purity, default: 0.99 |
| <code>ReportPoolSize</code> | default: TRUE |

Value

Named list of matrices: 'Corrected', 'Normalized', 'PoolBeforeDF', and 'PoolAfterDF'.

Examples

```
## Not run:  
nitrogen_isotope_correction(  
  formula = "C23H38N7O17P3S",  
  datamatrix = DataMatrix,  
  label = c(0, 1, 2, 3, 4, 5, 6, 7),  
  Resolution = 140000  
)  
  
## End(Not run)
```

`read_elmaven`*Natural Abundance correction for Carbon labeled samples*

Description

Natural Abundance correction for Carbon labeled samples

Usage

```
read_elmaven(  
  path,  
  sheet = NULL,  
  compound_database = NULL,  
  columns_to_skip = NULL,  
  filetype = NULL,  
  ...  
)
```

Arguments

| | |
|--------------------------------|---|
| <code>path</code> | Path to input file. |
| <code>sheet</code> | Name of sheet in xlsx file with columns 'compound', 'formula', 'isotopelabel', and one column per sample. Defaults to the first sheet. |
| <code>compound_database</code> | Path to compound database in csv format. Only used for classic MAVEN style input when formula is not specified. |
| <code>columns_to_skip</code> | Specify column heading to skip. All other columns not named 'compound', 'formula', and 'isotopelabel' will be assumed to be sample names. |
| <code>filetype</code> | Specify file type, default is to determine by file extension. |
| <code>...</code> | Pass additional parameters to readxl::read_excel |

Value

List containing three items: "original" data.frame which is result of read_excel, "cleaned" data.frame which with columns 'compound', 'formula', 'isotope_label', 'label_index', followed by columns for each sample, and "isotope" which is a character indicating the isotope

Examples

```
## Not run:  
read_elmaven_xlsx("ExcelFile", "Sheet1")  
  
## End(Not run)
```

Index

`accucor`, [2](#)

`accucor-package (accucor)`, [2](#)

`carbon_isotope_correction`, [3](#)

`clean_data_frame`, [4](#)

`deuterium_isotope_correction`, [4](#)

`natural_abundance_correction`, [2](#), [5](#)

`nitrogen_isotope_correction`, [7](#)

`read_elmaven`, [8](#)