Package 'isoorbi'

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Type Package

Title Process Orbitrap Iso Data

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BugReports https://github.com/isoverse/isoorbi/issues

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Imports tidyr (>= 1.2.0), dplyr (>= 1.0.0), magrittr (>= 2.0.0), rlang (>= 1.0.0), readr (>= 2.1.0), stringr (>= 1.4.0)

Suggests devtools, knitr, rmarkdown, testthat

Description Read and process isotopocule data from an Orbitrap Iso mass spectrometer. Hilkert et al. (2021) <doi:10.1021/acs.analchem.1c00944>.

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R topics documented:

`orbi_calculate_ratios` *Calculate isotopocule ratios*

Description

Ratio calculation between isotopocules and base peak defined by `orbi_define_basepeak`. Normally this function is not called directly by the user, but via the function `orbi_summarize_results`

Please note well: The formula used to calculate ion ratios matters! Do not simply use arithmetic mean. The best option may depend on the type of data you are processing (e.g., MS1 versus M+1 fragmentation).

Usage

```
orbi_calculate_ratios(
  numerator,
  denominator,
 ratio_method = c("mean", "sum", "median", "geometric_mean", "slope", "weighted_sum")
)
```

Arguments

`numerator`	Column(s) used as numerator; contains ion counts
`denominator`	Column used as denominator; contains ion counts
`ratio_method`	Method for computing the ratio

Details

Description of options for `ratio_method`:

- `mean`: arithmetic mean of ratios from individual scans.
- `sum`: sum of all ions of the numerator across all scans divided by the sum of all ions observed for the denominator across all scans.
- `geometric_mean`: geometric mean of ratios from individual scans.
- `slope`: The ratio is calculated using the slope obtained from a linear regression model that is weighted by the `numerator` `x`, using `stats::lm(x ~ y + 0, weights = x)`.
- `weighted_sum`: A derivative of the `sum` option. The weighing function ensures that each scan contributes equal weight to the ratio calculation, i.e. scans with more ions in the Orbitrap do not contribute disproportionately to the total `sum` of `x` and `y` that is used to calculate `x/y`.

Value

Calculated ratio between isotopocules defined as numerator(s) and denominator, using one of the ratio methods.

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package = "isoorbi")
df <- orbi_read_isox(file = fpath) %>%
                     orbi_simplify_isox() %>%
                     orbi_define_basepeak(basepeak_def = "M0")
ratios <- orbi_calculate_ratios(numerator = df$ions.incremental,
                          denominator = df$basepeak_ions,
                         ratio_method =  "sum")
```

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orbi_define_basepeak *Define and assign the base peak*

Description

`orbi_define_basepeak()` sets one isotopocule in the data frame as the base peak (ratio denominator)

Usage

```
orbi_define_basepeak(dataset, basepeak_def)
```

Arguments

`dataset`	A tibble from a `IsoX` output. Needs to contain columns for `filename`, `compound`, `scan.no`, `isotopocule`, `ions.incremental`.
`basepeak_def`	The isotopocule that gets defined as base peak, i.e. the denominator to calculate ratios

Value

Input data frame plus two columns called `basepeak` and `basepeak_ions`

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package = "isoorbi")
df <- orbi_read_isox(file = fpath) %>%
                     orbi_simplify_isox() %>%
                     orbi_define_basepeak(basepeak_def = "M0")
```

`orbi_filter_isox` *Basic generic filter for IsoX data*

Description

A basic filter function `orbi_filter_isox()` for file names, isotopocules, compounds and time ranges. Default value for all parameters is FALSE, i.e. no filter is applied.

Usage

```
orbi_filter_isox(
  dataset,
  filenames = FALSE,
  compounds = FALSE,
  isotopocules = FALSE,
  time_min = FALSE,
  time_max = FALSE
)
```

Arguments

`dataset`	The IsoX data to be filtered
`filenames`	Vector of file names to keep
`compounds`	Vector of compounds to keep
`isotopocules`	Vector of isotopocules to keep
`time_min`	Minimum retention time in minutes (`time.min`)
`time_max`	Maximum retention time in minutes (`time.min`)

Value

Filtered tibble

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package = "isoorbi")
df <- orbi_read_isox(file = fpath) %>%
orbi_simplify_isox() %>%
orbi_filter_isox(filenames = c("s3744"),
compounds = "HSO4-",
isotopocules = c("M0", "34S", "18O"),
time_min = FALSE,
time_max = FALSE)
```

orbi_filter_satellite_peaks

Filter to remove minor satellite peaks

Description

Remove minor signals (e.g., satellite peaks) that were reported by IsoX

Usage

```
orbi_filter_satellite_peaks(dataset)
```

Arguments

dataset	A data frame or tibble produced from IsoX data by orbi_simplify_isox()

Details

The orbi_filter_satellite_peaks() function removes minor signals for an isotopocule that have been reported by IsoX. These are often small satellite peaks generated by the Fourier transform.

If there are signal of high intensity or very many signals, this can indicate that the m/z and tolerance setting used for processing .raw files with IsoX were incorrect.

Value

Filtered data frame (tibble)

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package = "isoorbi")
df <- orbi_read_isox(file = fpath) %>%
orbi_simplify_isox() %>%
orbi_filter_satellite_peaks()
```

orbi_filter_scan_intensity

Filter to remove extreme scans

Description

The function orbi_filter_scan_intensity() removes extremely high and low intense scans based on TIC x injection time (i.e., ion intensity)

Usage

```
orbi_filter_scan_intensity(dataset, outlier_percent)
```

Arguments

`dataset`	Simplified IsoX dataset to have `TICxIT` outliers removed
`outlier_percent`	A number between 0 and 10. Remove this percentage of scans based on TIC multiplied by injection time.

Details

Function is intended to remove scans that are outliers. TIC multiplied by injection time serves as an estimate for the number of ions in the Orbitrap.

The filter is a basic truncation that removes `x %` of scans with the largest **and** `x %` of scans with the smallest ion estimates. Grouping is by columns `filename` and `compound`.

The input `dataset` is expected to have at least these 8 columns: `filename`, `scan.no`, `time.min`, `compound`, `isotopocule`, `ions.incremental`, `tic`, `it.ms`.

Value

Filtered tibble

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package = "isoorbi")
df <- orbi_read_isox(file = fpath) %>%
orbi_simplify_isox() %>%
orbi_filter_scan_intensity(outlier_percent = 1)
```

---

orbi_filter_weak_isotopocules

Filter to remove weak isotopocules

Description

The function `orbi_filter_weak_isotopocules()` removes isotopocules that are not consistently detected in most scans

Usage

```
orbi_filter_weak_isotopocules(dataset, min_percent)
```

Arguments

dataset	A simplified IsoX data frame to be processed
min_percent	A number between 0 and 90. Isotopocule must be observed in at least this percentage of scans (please note: the percentage is defined relative to the most commonly observed isotopocule of the compound)

Details

The input dataset is expected to have at least these 8 columns: filename, scan.no, time.min, compound, isotopocule, ions.incremental, tic, it.ms.

Value

Filtered tibble

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package = "isoorbi")
df <- orbi_read_isox(file = fpath) %>%
                     orbi_simplify_isox() %>%
                     orbi_filter_weak_isotopocules(min_percent = 2)
```

---

orbi_read_isox *Read IsoX file*

Description

Read an IsoX output file (.isox) into a tibble data frame

Usage

```
orbi_read_isox(file)
```

Arguments

file	Path to the .isox file

Details

Additional information on the columns:

- filename: name of the original Thermo .raw file processed by IsoX
- scan.no: scan number
- time.min: acquisition or retention time in minutes
- compound: name of the compound (e.g., NO3-)
- isotopocule: name of the isotopocule (e.g., 15N); called isotopolog in .isox

- `ions.incremental`: estimated number of ions, in increments since it is a calculated number
- `tic`: total ion current (TIC) of the scan
- `it.ms`: scan injection time (IT) in milli seconds (ms)

Value

A tibble containing at minimum the columns `filename`, `scan.no`, `time.min`, `compound`, `isotopocule`, `ions.incremental`, `tic`, `it.ms`

Examples

```
fpath <- system.file("extdata", "testfile_dual_inlet.isox", package="isoorbi")
df <- orbi_read_isox(file = fpath)
```

---

orbi_simplify_isox *Simplify IsoX data*

Description

Keep only columns that are directly relevant for isotopocule ratio analysis

Usage

```
orbi_simplify_isox(dataset)
```

Arguments

`dataset`	IsoX data that is to be simplified

Value

A tibble containing only the 8 columns: `filename`, `scan.no`, `time.min`, `compound`, `isotopocule`, `ions.incremental`, `tic`, `it.ms`.

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package="isoorbi")
df <- orbi_read_isox(file = fpath) %>% orbi_simplify_isox()
```

orbi_summarize_results *Generate the results table*

Description

Contains the logic to generate the results table. It passes the `ratio_method` parameter to the `orbi_calculate_ratios` function for ratio calculations.

Usage

```
orbi_summarize_results(dataset, ratio_method)
```

Arguments

`dataset`	A processed tibble produced from `IsoX` output
`ratio_method`	Method for computing the ratio

Details

Description of the output columns:

- `basepeak`: Isotopocule used as denominator in ratio calculation.
- `isotopocule`: Isotopocule used as numerator in ratio calculation.
- `ratio_sem`: Standard error of the mean for the ratio
- `number_of_scans`: Number of scans used for the final ratio calculation
- `minutes_to_1e6_ions`: Time in minutes it would take to observe 1 million ions of the `isotopocule` used as numerator of the ratio calculation.
- `shot_noise_permil`: Estimate of the shot noise (more correctly thermal noise) of the reported ratio in permil.
- `ratio_relative_sem_permil`: Relative standard error of the reported ratio in permil

Value

Returns a results table containing `filename`, `compound`, `basepeak`, `Isotopocule`, `ratio`, `ratio_sem`, `ratio_relative_sem_permil`, `shot_noise_permil`, `No.of.Scans`, `minutes_to_1e6_ions`

Examples

```
fpath <- system.file("extdata", "testfile_flow.isox", package = "isoorbi")
df <- orbi_read_isox(file = fpath) %>%
      orbi_simplify_isox() %>% orbi_define_basepeak(basepeak_def = "M0")  %>%
      orbi_summarize_results(ratio_method = "sum")
```

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