

Package ‘ProtExp’

May 2, 2017

Type Package
Title An Example Package for Proteomics Experiments
Version 1.0
Date 2017-05-02
Author NEU May Institute Advanced R Course
Description ProtExp is an example package illustrating
several R concepts for building packages
for analysis of proteomics experiments.
Maintainer Nobody <nobody@no.where>
License Artistic-2.0
LazyData true
Depends methods
Suggests tidyverse, knitr
VignetteBuilder knitr
RoxygenNote 6.0.1
NeedsCompilation no

R topics documented:

is_log_trans	1
normalize	2
ProtExp	3
twin	4
Index	5

is_log_trans	<i>Is a dataset log-transformed?</i>
--------------	--------------------------------------

Description

Returns TRUE if the data has been log-transformed and FALSE otherwise.

Usage

```
is_log_trans(object)

is_log_trans(object) <- value

## Default S3 method:
is_log_trans(object)

## Default S3 replacement method:
is_log_trans(object) <- value
```

Arguments

object	An object with data that may have been log-transformed.
--------	---

Details

This is an S3 generic function: methods can be defined for it by writing functions with the naming convention `is_log_trans.classname`. Functions should return `TRUE` or `FALSE`. The default method gets and sets the `is_log_trans` attribute.

Value

TRUE if the data has been log-transformed and FALSE otherwise.

Examples

```
x <- structure("test", is_log_trans = TRUE)
is_log_trans(x)
is_log_trans(x) <- FALSE
is_log_trans(x)
```

normalize	<i>Normalize a dataset</i>
-----------	----------------------------

Description

Performs normalization on an experimental dataset.

Usage

```
normalize(object, ...)

## S3 method for class 'ProtExp'
normalize(object, ..., by)
```

Arguments

object	An object with data to be normalized.
--------	---------------------------------------

Details

This is an S3 generic function: methods can be defined for it by writing functions with the naming convention `normalize.classname`. Functions should be appropriate for the experiment type.

`normalize.ProtExp` performs normalization on a `ProtExp` proteomics experiment dataset object using the median-of-medians method. It also performs log2-transformation on the intensities if the data has not already been log2-transformed.

Value

Another object of the same class with the normalized data.

ProtExp	<i>Proteomics Experiment</i>
---------	------------------------------

Description

Create a `ProtExp` object.

Usage

```
ProtExp(protein, feature, run, intensity, label, ..., is_log_trans = FALSE)
```

Arguments

<code>protein</code>	A character vector of protein names.
<code>feature</code>	A character vector of MS features.
<code>run</code>	A character or numeric vector of MS runs.
<code>intensity</code>	A numeric vector of MS intensities.
<code>label</code>	A character or factor of MS labels.
<code>...</code>	Additional columns.
<code>is_log_trans</code>	TRUE or FALSE indicating whether the intensities has been log2-transformed or not.

Details

`ProtExp` is a simple S3 class inheriting from `data.frame` for storing proteomics experiments. It expects columns named 'protein', 'feature', 'run', 'intensity', and 'label'. Additional columns are also allowed. A `ProtExp` object also has a `is_log_exp` attribute for tracking whether the intensities have been log2-transformed or not.

Value

object A `ProtExp` object.

twin

Twin DIA and SRM experiments

Description

DIA and SRM datasets from the same experiment. These datasets are subsets of the original datasets and have 33 proteins by DIA, and 39 proteins by SRM. The dataset includes 58 pairs of monozygotic (MZ) and dizygotic (DZ) twins, each measured at 2 time points, yielding $58 \times 2 \times 2 = 232$ MS runs. The variables are as follows:

Format

Two data frames with 103936 rows and 9 variables for `twin_dia` and 63104 rows and 9 variables for `twin_srm`.

Details

- `protein`. (chr) protein name.
- `feature`. (chr) combination of peptide, precursor charge state, fragment ion, and product charge state, separated by `_`.
- `run`. (chr) MS run identifier (R001-R232).
- `pair`. (int) pair identifier number (1-58).
- `zygosity`. (factor) zygosity (MZ, DZ).
- `subject`. (int) subject identifier number (1-116).
- `visit`. (int) time of visit (1, 2).
- `intensity_h`. (num) integrated feature intensity from light (L) channel.
- `intensity_l`. (num) integrated feature intensity from heavy (H, aka reference) channel.

Examples

```
data(twin)
head(twin_dia)
head(twin_srm)
```

Index

`is_log_trans`, [1](#)
`is_log_trans<- (is_log_trans)`, [1](#)
`normalize`, [2](#)
`ProtExp`, [3](#)
`twin`, [4](#)