# Package 'AlteredPQR'

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**Type** Package

**Title** Detection of Altered Protein Quantitative Relationships

**Version** 0.1.0

**Author** Marija Buljan [aut, cre]

**Maintainer** Marija Buljan <marija.buljan@empa.ch>

**Description** Inference of protein complex states from quantitative proteomics data. The package takes information on known stable protein interactions (i.e. protein components of the same complex) and assesses how protein quantitative ratios change between different conditions. It reports protein pairs for which relative protein quantities to each other have been significantly altered in the tested condition.

**License** GPL (>= 3)

**Encoding** UTF-8

**LazyData** true

**NeedsCompilation** no

**Depends** R (>= 3.5.0)

**Suggests** tools

**Repository** CRAN

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## R topics documented:

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AlteredPQR_RB                    *Identification of outlier log ratios in quantitative proteomic measure-*
                                 *ments for investigated protein pairs.*

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## Description

The function identifies outliers in protein pair log ratios compared to the reference set of measurements.

## Usage

```
AlteredPQR_RB (modif_z_score_threshold = 3.5, fraction_of_samples_threshold = 0.10,
modif = 1, filter_variable_in_ref_set = "NO", write_table = "NO", print_recomm = "NO",
quant_data_all_local = quant_data_all,
cols_with_reference_data_local = cols_with_reference_data)
```

## Arguments

modif_z_score_threshold

Numeric value defining a threshold to consider log ratio in the tested sample as a outlier.

fraction_of_samples_threshold

Numeric value defining a fraction of samples that need to be classified as outliers for the protein pair to be included in the results table.

modif                    Numeric value defining a modifier value that is used to idenify proteins in the pair that contributed to the outlier signal. The higher the variable 'modif', the higher the modified z score value the single protein needs to have (compared to its own values in the reference samples) to be considered as an outlier in at least half of the samples classified as outliers for the protein pair. Proteins classified as outliers in their own measuremnts are listed as 'driving the signal' in the reults table.

filter_variable_in_ref_set

Option (T or F) to exclude from the results table protein pairs that strongly varied in the reference samples.

write_table              Option (T or F) to save results table as a text file.

print_recomm             Option (T or F) to get information on the distribution of all modified z-scores in the test samples and recmmendation on the thresholds for the user defined qunatitative proteomics dataset.

quant_data_all_local

A data matrix with quantiative proteomics measurements in which rows represent uniprot protein identifiers, and columns samples.

cols_with_reference_data_local

Numeric vector with information on columns that contain reference data.

## Value

representative_pairs table

## Author(s)

Marija Buljan <marija.buljan@empa.ch>

## Examples

```
data("int_pairs", package = "AlteredPQR")
data("quant_data_all", package = "AlteredPQR")
cols_with_reference_data = 1:23
RepresentativePairs = AlteredPQR_RB()
```

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CorShift *Changes in correlation trends*

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## Description

The function identifies instances in which two proteins correlate strongly only in one of the two studied groups.

## Usage

```
CorShift(samplesA = samplesGroupA, samplesB = samplesGroupB, shift_threshold = 0.6,
 writeTable = FALSE, min_cor_in_samples = 0.6, cor_signif = 0.01,
 quant_data_all_local = quant_data_all, int_pairs_local = int_pairs)
```

## Arguments

samplesA          Numeric vector with information on column numbers for the samples in the first group for the comparison.

samplesB          Numeric vector with information on column numbers for the samples in the second group for the comparison.

shift_threshold
                  Numeric value defining a minimum thresold of the Pearson correlation value between the two sample groups in order for them to be included in the results table.

writeTable        Option (T or F) to save results table as a text file.

min_cor_in_samples
                  Numeric value defining a minimum Pearson correlation value of protein quantities, which is taken as a threshold to consider that two proteins correlate in either of the two compared groups.

cor_signif        Numeric value defining a maximum allowed p-value for the Pearson correlation, which is taken as a threshold to consider that quantiative measurements for the two proteins correlate significantly in either of the two compared groups.

quant_data_all_local
                  A data matrix with quantiative proteomics measurements in which rows represent uniprot protein identifiers, and columns samples.

int_pairs_local
                  A data matrix with two columns. Rows contain information on interacting protein pairs.

**Value**

cor_table table

**Author(s)**

Marija Buljan <marija.buljan@empa.ch>

**Examples**

```
data("int_pairs", package = "AlteredPQR")
data("quant_data_all", package = "AlteredPQR")
samplesGroupA = 1:23
samplesGroupB = (1+23):(23+18)
cor_results = CorShift()
```

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int_pairs                           *Protein pairs*

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**Description**

Protein pairs that can form stable interactions.

**Author(s)**

Marija Buljan <marija.buljan@empa.ch>

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quant_data_all              *Proteomic measurements data matrix*

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**Description**

Quantitative proteomics measurements; columns are samples, rows are proteins (Uniprot IDs).

**Author(s)**

Marija Buljan <marija.buljan@empa.ch>

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