Package ‘AlteredPQR’

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Type Package

Title Detection of Altered Protein Quantitative Relationships

Version 0.1.0

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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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Contents

`AlteredPQR_RB` *Identification of outlier log ratios in quantitative proteomic measurements for investigated protein pairs.*

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)

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Examples

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

`CorShift` *Changes in correlation trends*

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)

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Examples

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

`int_pairs` *Protein pairs*

Description

Protein pairs that can form stable interactions.

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`quant_data_all` *Proteomic measurements data matrix*

Description

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

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