Package 'statTarget'

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Type Package

Title Statistical Analysis of Metabolite Profile

Version 1.8.0

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Depends R (>= 3.3.0)

Imports randomForest,plyr,pdist,ROC,utils,grDevices,graphics,rrcov,stats, pls,impute,gWidgets2,gWidgets2RGtk2

VignetteBuilder knitr

Suggests testthat, BiocStyle, knitr, rmarkdown

Description An easy to use tool provides a graphical user interface for quality control based shift signal correction, integration of metabolomic data from multi-batch experiments, and the comprehensive statistic analysis in non-targeted or targeted metabolomics.

License GPL (>= 2)

URL https://github.com/13479776/statTarget

biocViews Metabolomics, MassSpectrometry, QualityControl, Regression, GUI

RoxygenNote 5.0.1

LazyData true

NeedsCompilation no

R topics documented:

statTarget-package *Statistical Analysis of Metabolite Profile*

Description

An easy to use tool provides graphical user interface for quality control based signal correction, integration of metabolomic data from multiple batches, and the comprehensive statistic analysis for non-targeted and targeted approaches.

Usage

```
statTarget()
```

Details

Package: statTarget

Type: package

Version: 1.5.6

Date: 2017-01-09

License: GPL (>= 2)

Value

A description of statTarget

Author(s)

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shiftCor *shiftCor for GUI*

Description

shiftCor provides the QC-RLS correction for large scale metabolomics.

Usage

```
shiftCor(samPeno, samFile, Frule = 0.8, QCspan = 0.75, degree = 2,
  imputeM = "KNN")
```

Arguments

samPeno	The file with the meta information including the sample name, batches, class and order.
samFile	The file with the expression information.
Frule	The cut-off value for missing value filter function.
QCspan	The smoothing parameter which controls the bias-variance tradeoff. if the QC-span is set at '0', the generalised cross-validation will be performed to avoid overfitting the observed data.
degree	Lets you specify local constant regression (i.e., the Nadaraya-Watson estimator, degree=0), local linear regression (degree=1), or local polynomial fits (degree=2, the default).
imputeM	The parameter for imputation method.(i.e., nearest neighbor averaging, "KNN"; minimum values for imputed variables, "min", median values for imputed variables (Group dependent) "median").

Value

An object of shiftCor

Examples

```
datpath <- system.file("extdata",package = "statTarget")
samPeno <- paste(datpath,"MTBLS79_sampleList.csv", sep="/")
samFile <- paste(datpath,"MTBLS79.csv", sep="/")
shiftCor(samPeno,samFile)
```

---

statAnalysis *statAnalysis for GUI*

Description

statAnalysis provides the statistical analysis for metabolomics data or others.

Usage

```
statAnalysis(file, Frule = 0.8, imputeM = "KNN", glog = TRUE,
  test.multi = TRUE, FDR = TRUE, nvarRF = 10, scaling = "Pareto",
  silt = 500, pcax = 1, pcay = 2, Labels = TRUE, upper.lim = 1.5,
  lower.lim = 0.5, sig.lim = 0.05)
```

Arguments

file	The file with the expression information.
Frule	The cut-off value for missing value filter function.
imputeM	The parameter for imputation method.(i.e., nearest neighbor averaging, "KNN"; minimum values for imputed variables, "min", median values for imputed variables (Group dependent) "median").
glog	Generalised logarithm (glog) transformation, with the default value TRUE.
test.multi	Multiple statistical analysis, with the default value TRUE.

FDR	The false discovery rate for conceptualizing the rate of type I errors in null hypothesis testing when conducting multiple comparisons.
nvarRF	The number of variables in Gini plot of Randomforest model (=< 100).
scaling	Scaling method before statistic analysis (PCA or PLS-DA). 'pareto', 'Pareto', 'p' or 'P' can be used for specifying the Pareto scaling. 'auto', 'Auto', 'auto', 'a' or 'A' can be used for specifying the Auto scaling (or unit variance scaling). 'vast', 'Vast', 'v' or 'V' can be used for specifying the vast scaling. 'range', 'Range', 'r' or 'R' can be used for specifying the Range scaling.
silt	The number of permutation times for PLS-DA model
pcax	Principal components in PCA model for the x-axis.
pcay	Principal components in PCA model for the y-axis.
Labels	Name labels for score plot of multiple statistical analysis
upper.lim	The up-regulated metabolites using Fold Changes cut off values in the Volcano plot.
lower.lim	The down-regulated metabolites using Fold Changes cut off values in the Volcano plot.
sig.lim	The significance level for metabolites in the Volcano plot.

Value

A object of statAnalysis

Examples

```
datpath <- system.file("extdata",package = "statTarget")
file <- paste(datpath,"data_example.csv", sep="/")
statAnalysis(file,nvarRF =5)
```

---

statTargetGUI *statTargetGUI for GUI*

Description

the statTarget GUI session. The Shift Correction and Statistical Analysis session being used by statTarget. Will restart statTarget if it died for some reason. Features of the package statTarget includes shift correction, typical quality control based robust LOESS signal correction (such as QC.RLSC); Data preprocessing, data descriptions, PCA, PLSDA, OPLSDA, VIP, ROC, random forest, odd ratio, Student T-test, Shapiro-Wilk normality test and Mann-Whitney tests; Data preprocessing includes 80-precent rule, log transformation, normalization. Data descriptions includes mean value, median value, sum, quartile, standard derivatives, etc.

Usage

```
statTargetGUI()
```

Value

The output of GUI

Author(s)

Hemi Luan hemi.luan@gmail.com

References

Dunn WB., et al. Nat Protoc. 2011, 6, pp1060. Luan H., et al. GigaScience 2015, 4, pp16. Luan H., et al. J. Proteome Res., 2015, 14, pp467.

Examples

```
if (interactive()) {statTargetGUI()}
```

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transCode *transCode for statTarget inputs*

Description

transCode is to generate statTarget inputs from Mass Spectrometry Data softwares, like XCMS.

Usage

```
transCode(data, type)
```

Arguments

data	A transCode objects. The output file from Mass Spectrometry Data softwares.
type	The output file formats from Mass Spectrometry Data software, including "XCMS" or "xcms",...; The softwares include XCMS (.tsv file generated from diffreport function), ...

Value

A list of inputs

Examples

```
datpath <- system.file("extdata",package = "statTarget")
data <- paste(datpath,"xcmsOutput.tsv", sep="/")
transCode(data,"xcms")
```

transX *transX for statTarget inputs*

Description

transX is to generate statTarget inputs from Mass Spectrometry Data softwares, like XCMS.

Usage

```
transX(data, type)
```

Arguments

data	A transX objects. The output file from Mass Spectrometry Data softwares.
type	The output file formats from Mass Spectrometry Data software, including "XCMS" or "xcms",...; The softwares include XCMS (.tsv file generated from diffreport function), ...

Value

A objects of transX

Examples

```
datpath <- system.file("extdata",package = "statTarget")
data <- paste(datpath,"xcmsOutput.tsv", sep="/")
transX(data,"xcms")
transCode(data,"xcms")
```

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