

Package ‘DAPAR’

October 17, 2017

Type Package

Title Tools for the Differential Analysis of Proteins Abundance with R

Version 1.8.7

Date 2017-05-29

Author Samuel Wieczorek [cre,aut],
Florence Combes [aut],
Thomas Burger [aut],
Cosmin Lazar [ctb],
Alexia Dorffer [ctb]

Maintainer Samuel Wieczorek <samuel.wieczorek@cea.fr>

Description This package contains a collection of functions for the
visualisation and the statistical analysis of proteomic data.

License Artistic-2.0

VignetteBuilder knitr

Depends R (>= 3.4)

Suggests BiocGenerics, Biobase, testthat, BiocStyle, Prostar

Imports MSnbase, RColorBrewer,stats,preprocessCore,Cairo,png,
lattice,reshape2,gplots,pcaMethods,ggplot2,
limma,knitr,tmvtnorm,norm,impute, imputeLCMD, doParallel,
parallel, foreach,grDevices, graphics, openxlsx, utils, cp4p
(>= 0.3.5), scales, Matrix, vioplot, imp4p (>= 0.3),
highcharter, DAPARdata

biocViews Proteomics, Normalization, Preprocessing, MassSpectrometry,
QualityControl, DataImport

NeedsCompilation no

RoxygenNote 6.0.1

R topics documented:

boxPlotD	3
BuildAdjacencyMatrix	4
BuildColumnToProteinDataset	5
compareNormalizationD	6
corrMatrixD	7
CountPep	7

createMSnset	8
CVDistD	9
deleteLinesFromIndices	10
densityPlotD	10
diffAna	11
diffAnaComputeFDR	12
diffAnaGetSignificant	13
diffAnaLimma	14
diffAnaSave	15
diffAnaVolcanoplot	16
diffAnaVolcanoplot_rCharts	17
diffAnaWelch	18
getIndicesConditions	19
getIndicesOfLinesToRemove	20
getNumberOf	20
getNumberOfEmptyLines	21
getPaletteForLabels	22
getPaletteForReplicates	22
getPourcentageOfMV	23
getProcessingInfo	24
getProteinsStats	24
GraphPepProt	25
heatmap.DAPAR	26
heatmapD	27
impute.pa2	27
limmaCompleteTest	28
MeanPeptides	29
mvFilter	30
mvFilterFromIndices	31
mvFilterGetIndices	32
mvHisto	33
mvImage	33
mvImputation	34
mvPerLinesHisto	35
mvPerLinesHistoPerCondition	35
mvTypePlot	36
normalizedD	37
normalizedD2	38
pepAggregate	39
proportionConRev	39
removeLines	40
SumPeptides	41
TopnPeptides	42
translatedRandomBeta	42
violinPlotD	43
wrapper.boxPlotD	44
wrapper.compareNormalizationD	45
wrapper.corrMatrixD	46
wrapper.CVDistD	46
wrapper.dapar.impute.mi	47
wrapper.densityPlotD	48
wrapper.diffAnaLimma	49

wrapper.diffAnaWelch	50
wrapper.heatmapD	50
wrapper.impute.pa	51
wrapper.impute.pa2	52
wrapper.mvHisto	53
wrapper.mvImage	53
wrapper.mvImputation	54
wrapper.mvPerLinesHisto	55
wrapper.mvPerLinesHistoPerCondition	55
wrapper.mvTypePlot	56
wrapper.normalized	57
wrapper.normalized2	57
wrapper.violinPlotD	58
wrapperCalibrationPlot	59
writeMSnsetToExcel	60

Index	61
--------------	-----------

boxPlotD	<i>Builds a boxplot from a dataframe</i>
----------	--

Description

Boxplot for quantitative proteomics data

Usage

```
boxPlotD(qData, dataForXAxis = NULL, labels = NULL,
group2Color = "Condition")
```

Arguments

qData	A dataframe that contains quantitative data.
dataForXAxis	A vector containing the types of replicates to use as X-axis. Available values are: Label, Analyt.Rep, Bio.Rep and Tech.Rep. Default is "Label".
labels	A vector of the conditions (labels) (one label per sample).
group2Color	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A boxplot

Author(s)

Florence Combes, Samuel Wiczorek

See Also

[densityPlotD](#)

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
types <- c("Label", "Analyt.Rep")
dataForXAxis <- Biobase::pData(Exp1_R25_pept)[, types]
labels <- Biobase::pData(Exp1_R25_pept)[, "Label"]
boxPlotD(qData, dataForXAxis, labels)
```

BuildAdjacencyMatrix *Function matrix of appartenance group*

Description

Method to create a binary matrix with proteins in columns and peptides in lines on a MSnSet object (peptides)

Usage

```
BuildAdjacencyMatrix(obj.pep, protID, unique = TRUE)
```

Arguments

obj.pep	An object (peptides) of class MSnbase .
protID	The name of proteins ID column
unique	A boolean to indicate whether only the unique peptides must be considered (TRUE) or if the shared peptides have to be integrated (FALSE).

Value

A binary matrix

Author(s)

Florence Combes, Samuel Wiczorek, Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], "Protein.group.IDs", TRUE)
```

BuildColumnToProteinDataset

creates a column for the protein dataset after agregation by using the previous peptide dataset.

Description

This function creates a column for the protein dataset after agregation by using the previous peptide dataset.

Usage

```
BuildColumnToProteinDataset(peptideData, matAdj, columnName, proteinNames)
```

Arguments

peptideData A data.frame of meta data of peptides. It is the fData of the MSnset object.

matAdj The adjacency matrix used to agregate the peptides data.

columnName The name of the column in fData(peptides_MSnset) that the user wants to keep in the new protein data.frame.

proteinNames The names of the protein in the new dataset (i.e. rownames)

Value

A vector

Author(s)

Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
protID <- "Protein.group.IDs"
M <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, FALSE)
data <- Biobase::fData(Exp1_R25_pept[1:1000])
protData <- pepAgregate(Exp1_R25_pept[1:1000], 'Protein_group_IDs', 'sum overall', M)
name <- "organism"
proteinNames <- rownames(Biobase::fData(protData))
BuildColumnToProteinDataset(data, M, name,proteinNames )
```

compareNormalizationD *Builds a plot from a dataframe*

Description

Plot to compare the quantitative proteomics data before and after normalization

Usage

```
compareNormalizationD(qDataBefore, qDataAfter, labelsForLegend = NULL,  
  indData2Show = NULL, group2Color = "Condition")
```

Arguments

qDataBefore	A dataframe that contains quantitative data before normalization.
qDataAfter	A dataframe that contains quantitative data after normalization.
labelsForLegend	A vector of the conditions (labels) (one label per sample).
indData2Show	A vector of the indices of the columns to show in the plot. The indices are those of indices of the columns in the data.frame qDataBefore.
group2Color	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A plot

Author(s)

Samuel Wiczorek

Examples

```
require(DAPARdata)  
data(Exp1_R25_pept)  
qDataBefore <- Biobase::exprs(Exp1_R25_pept)  
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]  
qDataAfter <- normalizeD(qDataBefore, labels, "Median Centering",  
  "within conditions")  
compareNormalizationD(qDataBefore, qDataAfter, labels)
```

corrMatrixD	<i>Displays a correlation matrix of the quantitative data of the exprs() table.</i>
-------------	---

Description

Correlation matrix based on a [MSnSet](#) object

Usage

```
corrMatrixD(qData, samplesData, gradientRate = 5)
```

Arguments

qData	A dataframe of quantitative data.
samplesData	A dataframe where lines correspond to samples and columns to the meta-data for those samples.
gradientRate	The rate parameter to control the exponential law for the gradient of colors

Value

A colored correlation matrix

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
samplesData <- Biobase::pData(Exp1_R25_pept)
corrMatrixD(qData, samplesData)
```

CountPep	<i>Compute the number of peptides used to aggregate proteins</i>
----------	--

Description

This function computes the number of peptides used to aggregate proteins.

Usage

```
CountPep(M)
```

Arguments

M	A "valued" adjacency matrix in which lines and columns correspond respectively to peptides and proteins.
---	--

Value

A vector of boolean which is the adjacency matrix but with NA values if they exist in the intensity matrix.

Author(s)

Alexia Dorffer

Examples

```
library(DAPARdata)
data(Exp1_R25_pept)
protID <- "Protein.group.IDs"
M <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, FALSE)
CountPep(M)
```

createMSnset

Creates an object of class [MSnSet](#) from text file

Description

Builds an object of class [MSnSet](#) from a single tabulated-like file for quantitative and meta-data and a dataframe for the samples description. It differs from the original [MSnSet](#) builder which requires three separated files tabulated-like quantitative proteomic data into a [MSnSet](#) object, including meta-data.

Usage

```
createMSnset(file, metadata = NULL, indExpData, indFData, indiceID = NULL,
             logData = FALSE, replaceZeros = FALSE, pep_prot_data = NULL)
```

Arguments

file	The name of a tab-separated file that contains the data.
metadata	A dataframe describing the samples (in lines).
indExpData	A vector of string where each element is the name of a column in designTable that have to be integrated in the fData() table of the MSnSet object.
indFData	The name of column in file that will be the name of rows for the exprs() and fData() tables
indiceID	The indice of the column containing the ID of entities (peptides or proteins)
logData	A boolean value to indicate if the data have to be log-transformed (Default is FALSE)
replaceZeros	A boolean value to indicate if the 0 and NaN values of intensity have to be replaced by NA (Default is FALSE)
pep_prot_data	A string that indicates whether the dataset is about peptides or proteins.

Value

An instance of class [MSnSet](#).

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
exprsFile <- system.file("extdata", "Exp1_R25_pept.txt",
  package="DAPARdata")
metadataFile <- system.file("extdata", "samples_Exp1_R25.txt",
  package="DAPARdata")
metadata = read.table(metadataFile, header=TRUE, sep="\t", as.is=TRUE)
indExpData <- c(56:61)
indFData <- c(1:55,62:71)
indiceID <- 64
createMSnset(exprsFile, metadata, indExpData, indFData, indiceID,
  pep_prot_data = "peptide")
```

CVDistD

Distribution of CV of entities

Description

Builds a densityplot of the CV of entities in the `exprs()` table of a object. The CV is calculated for each condition (Label) present in the dataset (see the slot 'Label' in the `pData()` table)

Usage

```
CVDistD(qData, labels = NULL)
```

Arguments

<code>qData</code>	A dataframe that contains quantitative data.
<code>labels</code>	A vector of the conditions (labels) (one label per sample).

Value

A density plot

Author(s)

Florence Combes, Samuel Wiczorek

See Also

[densityPlotD](#).

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]
CVDistD(Biobase::exprs(Exp1_R25_pept), labels)
```

deleteLinesFromIndices

Delete the lines in the matrix of intensities and the metadata table given their indice.

Description

Delete the lines of `exprs()` table identified by their indice.

Usage

```
deleteLinesFromIndices(obj, deleteThat = NULL, processText = "")
```

Arguments

`obj` An object of class `MSnSet` containing quantitative data.
`deleteThat` A vector of integers which are the indices of lines to delete.
`processText` A string to be included in the `MSnSet` object for log.

Value

An instance of class `MSnSet` that have been filtered.

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
deleteLinesFromIndices(Exp1_R25_pept, c(1:10))
```

densityPlotD

Builds a densityplot from a dataframe

Description

Densityplot of quantitative proteomics data over samples.

Usage

```
densityPlotD(qData, labelsForLegend = NULL, indData2Show = NULL,
  group2Color = "Condition")
```

Arguments

qData	A dataframe that contains quantitative data.
labelsForLegend	A vector of the conditions (labels) (one label per sample).
indData2Show	A vector of indices to show in densityplot. If NULL, then all labels are displayed.
group2Color	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A density plot

Author(s)

Florence Combes, Samuel Wiczorek

See Also

[boxPlotD](#), [CVDistD](#)

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
labels <- lab2Show <- Biobase::pData(Exp1_R25_pept)[,"Label"]
densityPlotD(qData, labels)
```

diffAna	<i>This function performs a differential analysis on an MSnSet object (adapted from limma)</i>
---------	--

Description

Performs a differential analysis on an [MSnSet](#) object, based on [limma](#) functions.

Usage

```
diffAna(qData, design)
```

Arguments

qData	A dataframe that contains quantitative data.
design	The design matrix as described in the limma package documentation

Value

A dataframe with the p-value and log(Fold Change) associated to each element (peptide/protein)

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept[1:1000])
design <- cbind(cond1=1,
  cond2 = rep(0,nrow(Biobase::pData(Exp1_R25_pept[1:1000])))
  rownames(design) <- rownames(Biobase::pData(Exp1_R25_pept[1:1000]))
  labels <- Biobase::pData(Exp1_R25_pept[1:1000])[, "Label"]
  indices <- getIndicesConditions(labels, "25fmol", "10fmol")
  design[indices$iCond2,2] <- 1
diffAna(qData, design)
```

diffAnaComputeFDR	<i>Computes the FDR corresponding to the p-values of the differential analysis using</i>
-------------------	--

Description

This function is a wrapper to the function `adjust.p` from the `cp4p` package. It returns the FDR corresponding to the p-values of the differential analysis. The FDR is computed with the function `p.adjust{stats}`.

Usage

```
diffAnaComputeFDR(data, threshold_PVal = 0, threshold_LogFC = 0,
  pi0Method = 1)
```

Arguments

data	The result of the differential analysis processed by <code>diffAna</code>
threshold_PVal	The threshold on p-value to distinguish between differential and non-differential data
threshold_LogFC	The threshold on log(Fold Change) to distinguish between differential and non-differential data
pi0Method	The parameter <code>pi0.method</code> of the method <code>adjust.p</code> in the package <code>cp4p</code>

Value

The computed FDR value (floating number)

Author(s)

Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
obj <- wrapper.mvImputation(Exp1_R25_pept[1:1000], "QRILC")
condition1 <- '25fmol'
condition2 <- '10fmol'
qData <- Biobase::exprs(obj)
samplesData <- Biobase::pData(obj)
labels <- Biobase::pData(obj)[,"Label"]
limma <- diffAnaLimma(qData,samplesData, labels, condition1, condition2)
diffAnaComputeFDR(limma)
```

`diffAnaGetSignificant` *Returns a MSnSet object with only proteins significant after differential analysis.*

Description

Returns a MSnSet object with only proteins significant after differential analysis.

Usage

```
diffAnaGetSignificant(obj)
```

Arguments

`obj` An object of class `MSnSet`.

Value

A MSnSet

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
condition1 <- "25fmol"
condition2 <- "10fmol"
resLimma <- wrapper.diffAnaLimma(Exp1_R25_pept[1:1000],
condition1, condition2)
obj <-diffAnaSave(Exp1_R25_pept[1:1000], resLimma, "limma",
condition1, condition2)
signif <- diffAnaGetSignificant(obj)
```

diffAnaLimma	<i>Performs differential analysis on an MSnSet object, calling the limma package functions</i>
--------------	--

Description

Method to perform differential analysis on an [MSnSet](#) object (calls the `limma` package function).

Usage

```
diffAnaLimma(qData, samplesData, labels, condition1, condition2)
```

Arguments

<code>qData</code>	A dataframe that contains quantitative data.
<code>samplesData</code>	A dataframe where lines correspond to samples and columns to the meta-data for those samples.
<code>labels</code>	A vector of the conditions (labels) (one label per sample).
<code>condition1</code>	A vector that contains the names of the conditions considered as condition 1
<code>condition2</code>	A vector that contains the names of the conditions considered as condition 2

Value

A dataframe as returned by the `limma` package

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
condition1 <- '25fmol'
condition2 <- '10fmol'
qData <- Biobase::exprs(Exp1_R25_pept[1:1000])
samplesData <- Biobase::pData(Exp1_R25_pept[1:1000])
labels <- Biobase::pData(Exp1_R25_pept[1:1000])[, "Label"]
diffAnaLimma(qData, samplesData, labels, condition1, condition2)
```

diffAnaSave	<i>Returns a MSnSet object with the results of the differential analysis performed with limma package.</i>
-------------	--

Description

This method returns a [MSnSet](#) object with the results of differential analysis.

Usage

```
diffAnaSave(obj, data, method = "limma", condition1, condition2,
            threshold_pVal = 1e-60, threshold_logFC = 0, fdr = 0,
            calibrationMethod = "pounds")
```

Arguments

obj	An object of class MSnSet .
data	The result of the differential analysis processed by diffAna
method	The method used for differential analysis. Available choices are : "limma", "Welch"
condition1	A vector containing the names (some values of the slot "Label" of <code>pData()</code> of the first condition.
condition2	A vector containing the names (some values of the slot "Label" of <code>pData()</code> of the second condition.
threshold_pVal	A float that indicates the threshold on p-value chosen to discriminate differential proteins.
threshold_logFC	A float that indicates the threshold on log(Fold Change) to discriminatedifferential proteins.
fdr	The FDR based on the values of <code>threshold_pVal</code> and <code>threshold_logFC</code>
calibrationMethod	The calibration method used to compute the calibration plot

Value

A [MSnSet](#)

Author(s)

Alexia Dorffer, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
condition1 <- '25fmol'
condition2 <- '10fmol'
limma <- wrapper.diffAnaLimma(Exp1_R25_pept[1:1000],
                             condition1, condition2)
obj <- diffAnaSave(Exp1_R25_pept[1:1000], limma, "limma",
                  condition1, condition2)
```

diffAnaVolcanoplot *Volcanoplot of the differential analysis*

Description

Plots a volcano plot after the differential analysis. Typically, the log of Fold Change is represented on the X-axis and the log10 of the p-value is drawn on the Y-axis. When the `threshold_pVal` and the `threshold_logFC` are set, two lines are drawn respectively on the y-axis and the X-axis to visually distinguish between differential and non differential data.

Usage

```
diffAnaVolcanoplot(logFC = NULL, pVal = NULL, threshold_pVal = 1e-60,  
  threshold_logFC = 0, conditions = NULL)
```

Arguments

<code>logFC</code>	A vector of the log(fold change) values of the differential analysis.
<code>pVal</code>	A vector of the p-value values returned by the differential analysis.
<code>threshold_pVal</code>	A floating number which represents the p-value that separates differential and non-differential data.
<code>threshold_logFC</code>	A floating number which represents the log of the Fold Change that separates differential and non-differential data.
<code>conditions</code>	A list of the names of condition 1 and 2 used for the differential analysis.

Value

A volcano plot

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)  
data(Exp1_R25_pept)  
condition1 <- '25fmol'  
condition2 <- '10fmol'  
data <- wrapper.diffAnaLimma(Exp1_R25_pept[1:1000], condition1, condition2)  
diffAnaVolcanoplot(data$logFC, data$P_Value)
```

`diffAnaVolcanoplot_rCharts`*Volcanoplot of the differential analysis*

Description

Plots an interactive volcano plot after the differential analysis. Typically, the log of Fold Change is represented on the X-axis and the log10 of the p-value is drawn on the Y-axis. When the `threshold_pVal` and the `threshold_logFC` are set, two lines are drawn respectively on the y-axis and the X-axis to visually distinguish between differential and non differential data. With the use of the package Highcharter, a customizable tooltip appears when the user put the mouse's pointer over a point of the scatter plot.

Usage

```
diffAnaVolcanoplot_rCharts(df, threshold_pVal = 1e-60, threshold_logFC = 0,
  conditions = NULL, clickFunction = NULL)
```

Arguments

<code>df</code>	A dataframe which contains the following slots : <code>x</code> : a vector of the log(fold change) values of the differential analysis, <code>y</code> : a vector of the p-value values returned by the differential analysis. <code>index</code> : a vector of the rownames of the data. This dataframe must have been built with the option <code>stringsAsFactors</code> set to <code>FALSE</code> . There may be additional slots which will be used to show informations in the tooltip. The name of these slots must begin with the prefix "tooltip_". It will be automatically removed in the plot.
<code>threshold_pVal</code>	A floating number which represents the p-value that separates differential and non-differential data.
<code>threshold_logFC</code>	A floating number which represents the log of the Fold Change that separates differential and non-differential data.
<code>conditions</code>	A list of the names of condition 1 and 2 used for the differential analysis.
<code>clickFunction</code>	A string that contains a JavaScript function used to show info from slots in df. The variable <code>this.index</code> refers to the slot named <code>index</code> and allows to retrieve the right row to show in the tooltip

Value

An interactive volcano plot

Author(s)

Samuel Wiczorek

Examples

```
library(highcharter)
require(DAPARdata)
data(Exp1_R25_pept)
obj <- Exp1_R25_pept[1:1000]
```

```

condition1 <- '25fmol'
condition2 <- '10fmol'
cond <- c(condition1, condition2)
keepThat <- mvFilterGetIndices(obj, 'wholeMatrix', '6')
obj <- mvFilterFromIndices(obj, keepThat,
  'Filtered with wholeMatrix (threshold = 6 ).')
data <- wrapper.diffAnaLinma(obj, condition1, condition2)
df <- data.frame(x=data$logFC,
  y = -log10(data$P_Value),
  index = as.character(rownames(obj)),
  stringsAsFactors = FALSE)
tooltipSlot <- c("Sequence", "Score")
df <- cbind(df, Biobase::fData(obj)[tooltipSlot])
colnames(df) <- gsub(".", "_", colnames(df), fixed=TRUE)
if (ncol(df) > 3){
  colnames(df)[4:ncol(df)] <-
  paste("tooltip_", colnames(df)[4:ncol(df)], sep="")
}
hc_clickFunction <- JS("function(event) {
  Shiny.onInputChange('eventPointClicked', [this.index]);}")
diffAnaVolcanoplot_rCharts(df, threshold_logFC = 1,
  threshold_pVal = 3,
  conditions = cond,
  clickFunction=hc_clickFunction)

```

diffAnaWelch	<i>Performs a differential analysis on a MSnSet object using the Welch t-test</i>
--------------	---

Description

Computes differential analysis on an [MSnSet](#) object, using the Welch t-test (`t.test{stats}`).

Usage

```
diffAnaWelch(qData, labels, condition1, condition2)
```

Arguments

qData	A dataframe that contains quantitative data.
labels	A vector of the conditions (labels) (one label per sample).
condition1	A vector containing the names of the conditions qData as condition 1
condition2	A vector containing the names of the conditions considered as condition 2

Value

A dataframe with two slots : P_Value (for the p-value) and logFC (the log of the Fold Change).

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
condition1 <- '25fmol'
condition2 <- '10fmol'
qData <- Biobase::exprs(Exp1_R25_pept[1:1000])
labels <- Biobase::pData(Exp1_R25_pept[1:1000])[, "Label"]
diffAnaWelch(qData, labels, condition1, condition2)
```

getIndicesConditions *Gets the conditions indices.*

Description

Returns a list for the two conditions where each slot is a vector of indices for the samples.

Usage

```
getIndicesConditions(labels, cond1, cond2)
```

Arguments

labels	A vector of strings containing the column "Label" of the pData().
cond1	A vector of Labels (a slot in the pData() table) for the condition 1.
cond2	A vector of Labels (a slot in the pData() table) for the condition 2.

Value

A list with two slots iCond1 and iCond2 containing respectively the indices of samples in the pData() table of the dataset.

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
labels <- Biobase::pData(Exp1_R25_pept)[, "Label"]
getIndicesConditions(labels, "25fmol", "10fmol")
```

`getIndicesOfLinesToRemove`*Get the indices of the lines to delete, based on a prefix string*

Description

This function returns the indice of the lines to delete, based on a prefix string

Usage

```
getIndicesOfLinesToRemove(obj, idLine2Delete = NULL, prefix = NULL)
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> .
<code>idLine2Delete</code>	The name of the column that correspond to the data to filter
<code>prefix</code>	A character string that is the prefix to find in the data

Value

A vector of integers.

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
getIndicesOfLinesToRemove(Exp1_R25_pept, "Potential.contaminant", prefix="+")
```

`getNumberOf`*Number of lines with prefix*

Description

Returns the number of lines, in a given column, where content matches the prefix.

Usage

```
getNumberOf(obj, name = NULL, prefix = NULL)
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> .
<code>name</code>	The name of a column.
<code>prefix</code>	A string

Value

An integer

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
getNumberOf(Exp1_R25_pept, "Potential.contaminant", "+")
```

`getNumberOfEmptyLines` *Returns the number of empty lines in the data*

Description

Returns the number of empty lines in a matrix.

Usage

```
getNumberOfEmptyLines(qData)
```

Arguments

qData A matrix corresponding to the quantitative data.

Value

An integer

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
getNumberOfEmptyLines(qData)
```

getPaletteForLabels *Palette for plots in DAPAR*

Description

Selects colors for the plots in DAPAR based on the different conditions in the dataset. The palette is derived from the brewer palette "Dark2" (see [RColorBrewer](#)).

Usage

```
getPaletteForLabels(labels)
```

Arguments

labels A vector of labels (strings).

Value

A palette designed for the data manipulated in DAPAR

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]
getPaletteForLabels(labels)
```

getPaletteForReplicates
 Palette for plot the replicates in DAPAR

Description

Selects colors for the plots in DAPAR based on the replicates in the dataset. The palette is derived from the brewer palette "Dark2" (see [RColorBrewer](#)).

Usage

```
getPaletteForReplicates(nColors)
```

Arguments

nColors The desired number of colors

Value

A palette designed for the data manipulated in DAPAR

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
n <- nrow(Biobase::pData(Exp1_R25_pept))
getPaletteForReplicates(n)
```

`getPourcentageOfMV` *Percentage of missing values*

Description

Returns the percentage of missing values in the quantitative data (`exprs()` table of the dataset).

Usage

```
getPourcentageOfMV(obj)
```

Arguments

`obj` An object of class `MSnSet`.

Value

A floating number

Author(s)

Florence Combes, Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
getPourcentageOfMV(Exp1_R25_pept)
```

getProcessingInfo *Returns the contains of the slot processing of an object of class MSnSet*

Description

Returns the contains of the slot processing of an object of class MSnSet.

Usage

```
getProcessingInfo(obj)
```

Arguments

obj An object (peptides) of class [MSnbase](#).

Value

The slot processing of obj@processingData

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
getProcessingInfo(Exp1_R25_pept)
```

getProteinsStats *computes the number of proteins that are only defined by specific peptides, shared peptides or a mixture of two.*

Description

This function computes the number of proteins that are only defined by specific peptides, shared peptides or a mixture of two.

Usage

```
getProteinsStats(matUnique, matShared)
```

Arguments

matUnique The adjacency matrix with only specific peptides.
matShared The adjacency matrix with both specific and shared peptides.

Value

A list

Author(s)

Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
protID <- "Protein.group.IDs"
MShared <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, FALSE)
MUnique <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, TRUE)
getProteinsStats(MUnique, MShared)
```

GraphPepProt

Function to create a histogram that shows the repartition of peptides w.r.t. the proteins

Description

Method to create a plot with proteins and peptides on a MSnSet object (peptides)

Usage

```
GraphPepProt(mat)
```

Arguments

mat An adjacency matrix.

Value

A histogram

Author(s)

Alexia Dorffer, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
mat <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], "Protein.group.IDs")
GraphPepProt(mat)
```

heatmap.DAPAR	<i>This function is inspired from the function heatmap.2 that displays quantitative data in the <code>exprs()</code> table of an object of class <code>MSnSet</code>. For more information, please refer to the help of the <code>heatmap.2</code> function.</i>
---------------	--

Description

Heatmap inspired by the `heatmap.2` function.

Usage

```
heatmap.DAPAR(x, col = heat.colors(100), srtCol = NULL, labCol = NULL,  
  labRow = NULL, key = TRUE, key.title = NULL, main = NULL,  
  ylab = NULL)
```

Arguments

<code>x</code>	A dataframe that contains quantitative data.
<code>col</code>	colors used for the image. Defaults to heat colors (<code>heat.colors</code>).
<code>srtCol</code>	angle of column labels, in degrees from horizontal
<code>labCol</code>	character vectors with column labels to use.
<code>labRow</code>	character vectors with row labels to use.
<code>key</code>	logical indicating whether a color-key should be shown.
<code>key.title</code>	main title of the color key. If set to NA no title will be plotted.
<code>main</code>	main title; default to none.
<code>ylab</code>	y-axis title; default to none.

Value

A heatmap

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)  
data(Exp1_R25_pept)  
obj <- mvFilter(Exp1_R25_pept, "wholeMatrix", 6)  
qData <- Biobase::exprs(obj)  
heatmap.DAPAR(qData)
```

heatmapD	<i>This function is a wrapper to heatmap.2 that displays quantitative data in the <code>exprs()</code> table of an object of class <code>MSnSet</code></i>
----------	--

Description

Heatmap of the quantitative proteomic data of a `MSnSet` object

Usage

```
heatmapD(qData, distance = "euclidean", cluster = "average",
         dendro = FALSE)
```

Arguments

qData	A dataframe that contains quantitative data.
distance	The distance used by the clustering algorithm to compute the dendrogram. See <code>help(heatmap.2)</code>
cluster	the clustering algorithm used to build the dendrogram. See <code>help(heatmap.2)</code>
dendro	A boolean to indicate if the dendrogram has to be displayed

Value

A heatmap

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
obj <- mvFilter(Exp1_R25_pept[1:1000], "wholeMatrix", 6)
qData <- Biobase::exprs(obj)
heatmapD(qData)
```

impute.pa2	<i>Missing values imputation from a <code>MSnSet</code> object</i>
------------	--

Description

This method is a variation to the function `impute.pa` from the package `imp4p`.

Usage

```
impute.pa2(tab, conditions, q.min = 0, q.norm = 3, eps = 0,
           distribution = "unif")
```

Arguments

tab	An object of class <code>MSnSet</code> .
conditions	xxxxxxxxxxxx
q.min	A quantile value of the observed values allowing defining the maximal value which can be generated. This maximal value is defined by the quantile q.min of the observed values distribution minus eps. Default is 0 (the maximal value is the minimum of observed values minus eps).
q.norm	A quantile value of a normal distribution allowing defining the minimal value which can be generated. Default is 3 (the minimal value is the maximal value minus $qn * \text{median}(\text{sd}(\text{observed values}))$ where sd is the standard deviation of a row in a condition).
eps	A value allowing defining the maximal value which can be generated. This maximal value is defined by the quantile q.min of the observed values distribution minus eps. Default is 0.
distribution	The type of distribution used. Values are unif or beta.

Value

The object obj which has been imputed

Author(s)

Thomas Burger, Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.impute.pa2(Exp1_R25_pept[1:1000], distribution="beta")
```

limmaCompleteTest *Computes a hierarchical differential analysis*

Description

This function is a limmaCompleteTest

Usage

```
limmaCompleteTest(qData, Conditions, RepBio, RepTech, Contrast = 1)
```

Arguments

qData	A matrix of quantitative data, without any missing values.
Conditions	A vector of factor which indicates the name of the biological condition for each replicate.
RepBio	A vector of factor which indicates the number of the bio rep for each replicate.
RepTech	A vector of factor which indicates the number of the tech rep for each replicate.
Contrast	Indicates if the test consists of the comparison of each biological condition versus each of the other ones (Contrast=1; for example H0:"C1=C2" vs H1:"C1!=C2", etc.) or each condition versus all others (Contrast=2; e.g. H0:"C1=(C2+C3)/2" vs H1:"C1!=(C2+C3)/2", etc. if there are three conditions).

Value

fdsfdgfdg

Author(s)

Quentin Giai-Gianetto

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
obj <- wrapper.mvImputation(Exp1_R25_pept[1:1000], "QRILC")
condition1 <- '25fmol'
condition2 <- '10fmol'
qData <- Biobase::exprs(obj)
RepBio <- RepTech <- factor(1:6)
conds <- factor(c(rep(condition1, 3), (rep(condition2, 3))))
limma <- limmaCompleteTest(qData,conds,RepBio, RepTech)
```

MeanPeptides

Compute the intensity of proteins as the mean of the intensities of their peptides.

Description

This function computes the intensity of proteins as the mean of the intensities of their peptides.

Usage

```
MeanPeptides(matAdj, expr)
```

Arguments

matAdj An adjacency matrix in which lines and columns correspond respectively to peptides and proteins.

expr A matrix of intensities of peptides

Value

A matrix of intensities of proteins

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
protID <- "Protein.group.IDs"
matAdj <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, FALSE)
MeanPeptides(matAdj, Biobase::exprs(Exp1_R25_pept[1:1000]))
```

`mvFilter`*Filter lines in the matrix of intensities w.r.t. some criteria*

Description

Filters the lines of `exprs()` table with conditions on the number of missing values. The user chooses the minimum amount of intensities that is acceptable and the filter delete lines that do not respect this condition. The condition may be on the whole line or condition by condition.

Usage

```
mvFilter(obj, type, th, processText = NULL)
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> containing quantitative data.
<code>type</code>	Method used to choose the lines to delete. Values are : "none", "wholeMatrix", "allCond", "atLeastOneCond"
<code>th</code>	An integer value of the threshold
<code>processText</code>	A string to be included in the <code>MSnSet</code> object for log.

Details

The different methods are : "wholeMatrix": given a threshold `th`, only the lines that contain at least `th` values are kept. "allCond": given a threshold `th`, only the lines which contain at least `th` values for each of the conditions are kept. "atLeastOneCond": given a threshold `th`, only the lines that contain at least `th` values, and for at least one condition, are kept.

Value

An instance of class `MSnSet` that have been filtered.

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
mvFilter(Exp1_R25_pept, "wholeMatrix", 2)
```

mvFilterFromIndices *Filter lines in the matrix of intensities w.r.t. some criteria*

Description

Filters the lines of `exprs()` table with conditions on the number of missing values. The user chooses the minimum amount of intensities that is acceptable and the filter delete lines that do not respect this condition. The condition may be on the whole line or condition by condition.

Usage

```
mvFilterFromIndices(obj, keepThat = NULL, processText = "")
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> containing quantitative data.
<code>keepThat</code>	A vector of integers which are the indices of lines to keep.
<code>processText</code>	A string to be included in the <code>MSnSet</code> object for log.

Details

The different methods are : "wholeMatrix": given a threshold `th`, only the lines that contain at least `th` values are kept. "allCond": given a threshold `th`, only the lines which contain at least `th` values for each of the conditions are kept. "atLeastOneCond": given a threshold `th`, only the lines that contain at least `th` values, and for at least one condition, are kept.

Value

An instance of class `MSnSet` that have been filtered.

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
mvFilterFromIndices(Exp1_R25_pept, c(1:10))
```

mvFilterGetIndices *Filter lines in the matrix of intensities w.r.t. some criteria*

Description

Returns the indices of the lines of `exprs()` table to delete w.r.t. the conditions on the number of missing values. The user chooses the minimum amount of intensities that is acceptable and the filter delete lines that do not respect this condition. The condition may be on the whole line or condition by condition.

Usage

```
mvFilterGetIndices(obj, type, th)
```

Arguments

obj	An object of class MSnSet containing quantitative data.
type	Method used to choose the lines to delete. Values are : "none", "wholeMatrix", "allCond", "atLeastOneCond"
th	An integer value of the threshold

Details

The different methods are : "wholeMatrix": given a threshold `th`, only the lines that contain at least `th` values are kept. "allCond": given a threshold `th`, only the lines which contain at least `th` values for each of the conditions are kept. "atLeastOneCond": given a threshold `th`, only the lines that contain at least `th` values, and for at least one condition, are kept.

Value

An vector of indices that correspond to the lines to keep.

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
mvFilterGetIndices(Exp1_R25_pept, "wholeMatrix", 2)
```

mvHisto	<i>Histogram of missing values</i>
---------	------------------------------------

Description

This method plots a histogram of missing values.

Usage

```
mvHisto(qData, samplesData, labels, indLegend = "auto", showValues = FALSE)
```

Arguments

qData	A dataframe that contains quantitative data.
samplesData	A dataframe where lines correspond to samples and columns to the meta-data for those samples.
labels	A vector of the conditions (labels) (one label per sample).
indLegend	The indices of the column name's in pData() tab
showValues	A logical that indicates wether numeric values should be drawn above the bars.

Value

A histogram

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
samplesData <- Biobase::pData(Exp1_R25_pept)
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]
mvHisto(qData, samplesData, labels, indLegend="auto", showValues=TRUE)
```

mvImage	<i>Heatmap of missing values</i>
---------	----------------------------------

Description

Plots a heatmap of the quantitative data. Each column represent one of the conditions in the object of class [MsnSet](#) and the color is proportional to the mean of intensity for each line of the dataset. The lines have been sorted in order to visualize easily the different number of missing values. A white square is plotted for missing values.

Usage

```
mvImage(qData, labels)
```

Arguments

qData A dataframe that contains quantitative data.
labels A vector of the conditions (labels) (one label per sample).

Value

A heatmap

Author(s)

Samuel Wieczorek, Thomas Burger

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]
mvImage(qData, labels)
```

mvImputation

Missing values imputation from a matrix

Description

This method is a wrapper to the `imputeLCMD` package adapted to a matrix.

Usage

```
mvImputation(qData, method)
```

Arguments

qData A dataframe that contains quantitative data.
method The imputation method to be used. Choices are QRILC, KNN, BPCA and MLE.

Value

The matrix imputed

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)[1:1000]
mvImputation(qData, "QRILC")
```

mvPerLinesHisto	<i>Bar plot of missing values per lines</i>
-----------------	---

Description

This method plots a bar plot which represents the distribution of the number of missing values (NA) per lines (ie proteins).

Usage

```
mvPerLinesHisto(qData, samplesData, indLegend = "auto", showValues = FALSE)
```

Arguments

qData	A dataframe that contains the data to plot.
samplesData	A dataframe which contains informations about the replicates.
indLegend	The indice of the column name's in pData() tab
showValues	A logical that indicates wether numeric values should be drawn above the bars.

Value

A bar plot

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
samplesData <- Biobase::pData(Exp1_R25_pept)
mvPerLinesHisto(qData, samplesData)
```

mvPerLinesHistoPerCondition	<i>Bar plot of missing values per lines and per condition</i>
-----------------------------	---

Description

This method plots a bar plot which represents the distribution of the number of missing values (NA) per lines (ie proteins) and per conditions.

Usage

```
mvPerLinesHistoPerCondition(qData, samplesData, indLegend = "auto",
  showValues = FALSE)
```

Arguments

qData	A dataframe that contains quantitative data.
samplesData	A dataframe where lines correspond to samples and columns to the meta-data for those samples.
indLegend	The indice of the column name's in pData() tab
showValues	A logical that indicates wether numeric values should be drawn above the bars.

Value

A bar plot

Author(s)

Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
samplesData <- Biobase::pData(Exp1_R25_pept)
mvPerLinesHistoPerCondition(qData, samplesData)
```

mvTypePlot

Distribution of missing values with respect to intensity values

Description

This method plots a scatter plot which represents the distribution of missing values. The colors correspond to the different conditions (slot Label in in the dataset of class `MSnSet`). The x-axis represent the mean of intensity for one condition and one entity in the dataset (i. e. a protein) whereas the y-axis count the number of missing values for this entity and the considered condition. The data have been jittered for an easier vizualisation.

Usage

```
mvTypePlot(qData, labels, threshold = 0)
```

Arguments

qData	A dataframe that contains quantitative data.
labels	A vector of the conditions (labels) (one label per sample).
threshold	An integer for the intensity that delimits MNAR and MCAR missing values.

Value

A scatter plot

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept)
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]
mvTypePlot(qData, labels, threshold=0)
```

normalizedD

*Normalisation***Description**

Provides several methods to normalize data from a matrix. They are organized in four main families : Strong Rescaling, Median Centering, Mean Centering, Mean CenteringScaling. For the first family, two sub-categories are available : the sum by columns and the quantiles method. For the three other families, two categories are available : "overall" which means that the value for each protein (ie line in the expression data tab) is computed over all the samples ; "within conditions" which means that the value for each protein (ie line in the matrix) is computed condition by condition.

Usage

```
normalizedD(qData, labels, family, method)
```

Arguments

qData	A dataframe that contains quantitative data.
labels	A vector of strings containing the column "Label" of the pData().
family	One of the following : Global Alignment, Median Centering, Mean Centering, Mean Centering Scaling.
method	"Overall" or "within conditions".

Value

A matrix normalized

Author(s)

Florence Combes, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept[1:1000])
labels <- Biobase::pData(Exp1_R25_pept[1:1000])[,"Label"]
normalizedD(qData, labels, "Median Centering", "within conditions")
```

normalizeD2

*Normalisation***Description**

Provides several methods to normalize data from a matrix. They are organized in four main families : Strong Rescaling, Median Centering, Mean Centering, Mean CenteringScaling. For the first family, two sub-categories are available : the sum by columns and the quantiles method. For the three other families, two categories are available : "Overall" which means that the value for each protein (ie line in the expression data tab) is computed over all the samples ; "within conditions" which means that the value for each protein (ie line in the matrix) is computed condition by condition.

Usage

```
normalizeD2(qData, labels, method, type, scaling = FALSE, quantile = 0.15)
```

Arguments

qData	A dataframe that contains quantitative data.
labels	A vector of strings containing the column "Label" of the pData().
method	One of the following : Global Alignment, Quantile Centering, Mean Centering.
type	For the method "Global Alignment", the parameters are: "sum by columns": operates on the original scale (not the log2 one) and propose to normalize each abundance by the total abundance of the sample (so as to focus on the analyte proportions among each sample). "Alignment on all quantiles": proposes to align the quantiles of all the replicates; practically it amounts to replace abundances by order statistics. For the two other methods, the parameters are "overall" (shift all the sample distributions at once) or "within conditions" (shift the sample distributions within each condition at a time).
scaling	A boolean that indicates if the variance of the data have to be forced to unit (variance reduction) or not.
quantile	A float that corresponds to the quantile used to align the data.

Value

A matrix normalized

Author(s)

Samuel Wiczorek, Thomas Burger

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
qData <- Biobase::exprs(Exp1_R25_pept[1:1000])
labels <- Biobase::pData(Exp1_R25_pept[1:1000])[,"Label"]
normalizeD2(qData, labels, "Quantile Centering", "within conditions", quantile = 0.15)
```

pepAggregate *Function aggregate peptides to proteins*

Description

Method to aggregate with a method peptides to proteins on a MSnSet object (peptides)

Usage

```
pepAggregate(obj.pep, protID, method = "sum overall", matAdj = NULL,
             n = NULL)
```

Arguments

obj.pep	An object (peptides) of class MSnbase .
protID	The name of proteins ID column
method	The method used to aggregate the peptides into proteins. Values are "sum", "mean" or "sum on top n" : do the sum / mean of intensity on all peptides belonging to proteins. Default is "sum"
matAdj	An adjacency matrix
n	The number of peptides considered for the aggregation.

Value

An object of class [MSnbase](#) with proteins

Author(s)

Alexia Dorffer, Samuel Wiczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
protID <- "Protein.group.IDs"
mat <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, TRUE)
pepAggregate(Exp1_R25_pept[1:1000], protID, "sum overall", mat)
```

proportionConRev *Barplot of proportion of contaminants and reverse*

Description

Plots a barplot of proportion of contaminants and reverse

Usage

```
proportionConRev(obj, idContaminants = NULL, prefixContaminants = NULL,
                 idReverse = NULL, prefixReverse = NULL)
```

Arguments

obj An object of class [MSnSet](#).
idContaminants The name of a column of Contaminants
prefixContaminants The prefix to identify contaminants
idReverse The name of a column of Reverse
prefixReverse The prefix to identify Reverse

Value

A barplot

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
pref <- "+"
proportionConRev(Exp1_R25_pept, "Potential.contaminant", pref,
"Reverse", pref)
```

removeLines	<i>Removes lines in the dataset based on a prefix string.</i>
-------------	---

Description

This function removes lines in the dataset based on a prefix string.

Usage

```
removeLines(obj, idLine2Delete = NULL, prefix = NULL)
```

Arguments

obj An object of class [MSnSet](#).
idLine2Delete The name of the column that correspond to the data to filter
prefix A character string that is the prefix to find in the data

Value

An object of class [MSnSet](#).

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
removeLines(Exp1_R25_pept, "Potential.contaminant")
removeLines(Exp1_R25_pept, "Reverse")
```

SumPeptides	<i>Compute the intensity of proteins with the sum of the intensities of their peptides.</i>
-------------	---

Description

This function computes the intensity of proteins based on the sum of the intensities of their peptides.

Usage

```
SumPeptides(matAdj, expr)
```

Arguments

matAdj	An adjacency matrix in which lines and columns correspond respectively to peptides and proteins.
expr	A matrix of intensities of peptides

Value

A matrix of intensities of proteins

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
protID <- "Protein.group.IDs"
M <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, FALSE)
SumPeptides(M, Biobase::exprs(Exp1_R25_pept[1:1000]))
```

TopnPeptides	<i>Compute the intensity of proteins as the sum of the intensities of their n best peptides.</i>
--------------	--

Description

This function computes the intensity of proteins as the sum of the intensities of their n best peptides.

Usage

```
TopnPeptides(matAdj, expr, n)
```

Arguments

matAdj	An adjacency matrix in which lines and columns correspond respectively to peptides and proteins.
expr	A matrix of intensities of peptides
n	The maximum number of peptides used to aggregate a protein.

Value

A matrix of intensities of proteins

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
protID <- "Protein.group.IDs"
matAdj <- BuildAdjacencyMatrix(Exp1_R25_pept[1:1000], protID, FALSE)
TopnPeptides(matAdj, Biobase::exprs(Exp1_R25_pept[1:1000]), 3)
```

translatedRandomBeta	xxxxxxx
----------------------	---------

Description

This method xxxxxxxxxxxx

Usage

```
translatedRandomBeta(n, min, max, param1 = 3, param2 = 1)
```

Arguments

n	An integer which is the number of simulation (same as in rbeta)
min	An integer that corresponds to the lower bound of the interval
max	An integer that corresponds to the upper bound of the interval
param1	An integer that is the first parameter of rbeta function.
param2	An integer that is second parameter of rbeta function.

Value

A vector of n simulated values

Author(s)

Thomas Burger

Examples

```
translatedRandomBeta(1000, 5, 10, 1, 1)
```

violinPlotD

Builds a violinplot from a dataframe

Description

ViolinPlot for quantitative proteomics data

Usage

```
violinPlotD(qData, dataForXAxis = NULL, labels = NULL,
            group2Color = "Condition")
```

Arguments

qData	A dataframe that contains quantitative data.
dataForXAxis	A vector containing the types of replicates to use as X-axis. Available values are: Label, Analyt.Rep, Bio.Rep and Tech.Rep. Default is "Label".
labels	A vector of the conditions (labels) (one label per sample).
group2Color	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A violinplot

Author(s)

Florence Combes, Samuel Wiczorek

See Also[densityPlotD](#)**Examples**

```
require(DAPARdata)
data(Exp1_R25_pept)
library(vioplot)
qData <- Biobase::exprs(Exp1_R25_pept)
types <- c("Label", "Analyt.Rep")
dataForXAxis <- Biobase::pData(Exp1_R25_pept)[, types]
labels <- Biobase::pData(Exp1_R25_pept)[, "Label"]
violinPlotD(qData, dataForXAxis, labels)
```

`wrapper.boxPlotD`*Wrapper to the `boxplotD` function on an object `MSnSet`*

Description

This function is a wrapper for using the `boxPlotD` function with objects of class `MSnSet`

Usage

```
wrapper.boxPlotD(obj, dataForXAxis = "Label", group2Color = "Condition")
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> .
<code>dataForXAxis</code>	A vector of strings containing the names of columns in <code>pData()</code> to print labels on X-axis (Default is "Label").
<code>group2Color</code>	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A boxplot

Author(s)

Florence Combes, Samuel Wiczorek

See Also[wrapper.densityPlotD](#)**Examples**

```
require(DAPARdata)
data(Exp1_R25_pept)
types <- c("Label", "Analyt.Rep")
wrapper.boxPlotD(Exp1_R25_pept, types)
```

wrapper.compareNormalizationD
Builds a plot from a dataframe

Description

Wrapper to the function that plot to compare the quantitative proteomics data before and after normalization

Usage

```
wrapper.compareNormalizationD(objBefore, objAfter, labelsForLegend = NULL,  
  indData2Show = NULL, group2Color = "Condition")
```

Arguments

objBefore	A dataframe that contains quantitative data before normalization.
objAfter	A dataframe that contains quantitative data after normalization.
labelsForLegend	A vector of the conditions (labels) (one label per sample).
indData2Show	A vector of the indices of the columns to show in the plot. The indices are those of indices of the columns in the data.frame qDataBefore.
group2Color	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A plot

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)  
data(Exp1_R25_pept)  
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]  
objAfter <- wrapper.normalized(Exp1_R25_pept, "Median Centering",  
  "within conditions")  
wrapper.compareNormalizationD(Exp1_R25_pept, objAfter, labels)
```

wrapper.corrMatrixD *Displays a correlation matrix of the quantitative data of the exprs() table*

Description

Builds a correlation matrix based on a [MSnSet](#) object.

Usage

```
wrapper.corrMatrixD(obj, rate = 5)
```

Arguments

obj An object of class [MSnSet](#).
rate A float that defines the gradient of colors.

Value

A colored correlation matrix

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.corrMatrixD(Exp1_R25_pept)
```

wrapper.CVDistD *Distribution of CV of entities*

Description

Builds a densityplot of the CV of entities in the exprs() table of an object [MSnSet](#). The variance is calculated for each condition (Label) present in the dataset (see the slot 'Label' in the pData() table).

Usage

```
wrapper.CVDistD(obj)
```

Arguments

obj An object of class [MSnSet](#).

Value

A density plot

Author(s)

Alexia Dorffer

See Also[wrapper.densityPlotD](#)**Examples**

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.CVDistD(Exp1_R25_pept)
```

 wrapper.dapar.impute.mi

Missing values imputation using the LSImpute algorithm.

Description

This method is a wrapper to the function `impute.mi` of the package `imp4p` adapted to an object of class `MSnSet`.

Usage

```
wrapper.dapar.impute.mi(obj, nb.iter = 3, nknn = 15, selec = 600,
  siz = 500, weight = 1, ind.comp = 1, progress.bar = TRUE,
  x.step.mod = 300, x.step.pi = 300, nb.rei = 100, method = 4,
  gridsize = 300, q = 0.95, q.min = 0, q.norm = 3, eps = 0,
  methodi = "slsa", lapala = TRUE, distribution = "unif")
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> .
<code>nb.iter</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>nknn</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>selec</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>siz</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>weight</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>ind.comp</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>progress.bar</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>x.step.mod</code>	Same as the function <code>estim.mix</code> in the package <code>imp4p</code>
<code>x.step.pi</code>	Same as the function <code>estim.mix</code> in the package <code>imp4p</code>
<code>nb.rei</code>	Same as the function <code>estim.mix</code> in the package <code>imp4p</code>
<code>method</code>	Same as the function <code>estim.mix</code> in the package <code>imp4p</code>
<code>gridsize</code>	Same as the function <code>estim.mix</code> in the package <code>imp4p</code>
<code>q</code>	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
<code>q.min</code>	Same as the function <code>impute.pa</code> in the package <code>imp4p</code>

q.norm	Same as the function <code>impute.pa</code> in the package <code>imp4p</code>
eps	Same as the function <code>impute.pa</code> in the package <code>imp4p</code>
methodi	Same as the function <code>mi.mix</code> in the package <code>imp4p</code>
lapala	xxxxxxxxxxx
distribution	xxxxxxxxxxx

Value

The `exprs(obj)` matrix with imputed values instead of missing values.

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
dat <- mvFilter(Exp1_R25_pept[1:1000], type="allCond", th = 1)
dat <- wrapper.dapar.impute.mi(dat, nb.iter=1)
```

`wrapper.densityPlotD` *Builds a densityplot from an object of class `MSnSet`*

Description

This function is a wrapper for using the `densityPlotD` function with objects of class `MSnSet`

Usage

```
wrapper.densityPlotD(obj, labelsForLegend = NULL, indData2Show = NULL,
  group2Color = "Condition")
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> .
<code>labelsForLegend</code>	A vector of labels to show in densityplot.
<code>indData2Show</code>	A vector of the indices of the columns to show in the plot. The indices are those of indices of the columns in the data frame <code>qDataBefore</code> in the density plot.
<code>group2Color</code>	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A density plot

Author(s)

Alexia Dorffer

See Also

[wrapper.boxPlotD](#), [wrapper.CVDistD](#)

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
labels <- Biobase::pData(Exp1_R25_pept)[,"Label"]
wrapper.densityPlotD(Exp1_R25_pept, labels)
```

`wrapper.diffAnaLimma` *Performs differential analysis on an MSnSet object, calling the limma package functions*

Description

Method to perform differential analysis on a [MSnSet](#) object (calls the limma package function).

Usage

```
wrapper.diffAnaLimma(obj, condition1, condition2)
```

Arguments

`obj` An object of class [MSnSet](#).

`condition1` A vector that contains the names of the conditions considered as condition 1.

`condition2` A vector that contains the names of the conditions considered as condition 2.

Value

A dataframe as returned by the limma package

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
condition1 <- '25fmol'
condition2 <- '10fmol'
wrapper.diffAnaLimma(Exp1_R25_pept[1:1000], condition1, condition2)
```

`wrapper.diffAnaWelch` *Performs a differential analysis on a [MSnSet](#) object using the Welch t-test*

Description

Computes differential analysis on a [MSnSet](#) object, using the Welch t-test (`t.test{stats}`).

Usage

```
wrapper.diffAnaWelch(obj, condition1, condition2)
```

Arguments

`obj` An object of class [MSnSet](#).
`condition1` A vector containing the names of the conditions considered as condition 1.
`condition2` A vector containing the names of the conditions considered as condition 2.

Value

A dataframe with two slots : `P_Value` (for the p-value) and `logFC` (the log of the Fold Change).

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
condition1 <- '25fmol'
condition2 <- '10fmol'
wrapper.diffAnaWelch(Exp1_R25_pept[1:1000], condition1, condition2)
```

`wrapper.heatmapD` *This function is a wrapper to [heatmap.2](#) that displays quantitative data in the `exprs()` table of an object of class [MSnSet](#)*

Description

Builds a heatmap of the quantitative proteomic data of a [MSnSet](#) object.

Usage

```
wrapper.heatmapD(obj, distance = "euclidean", cluster = "average",
  dendro = FALSE)
```

Arguments

obj	An object of class MSnSet .
distance	The distance used by the clustering algorithm to compute the dendrogram. See <code>help(heatmap.2)</code> .
cluster	the clustering algorithm used to build the dendrogram. See <code>help(heatmap.2)</code>
dendro	A boolean to indicate if the dendrogram has to be displayed

Value

A heatmap

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
obj <- mvFilter(Exp1_R25_pept[1:1000], "wholeMatrix", 6)
wrapper.heatmapD(obj)
```

wrapper.impute.pa *Imputation of peptides having no values in a biological condition.*

Description

This method is a wrapper to the function `impute.pa` of the package `imp4p` adapted to an object of class [MSnSet](#).

Usage

```
wrapper.impute.pa(obj, q.min = 0.025)
```

Arguments

obj	An object of class MSnSet .
q.min	Same as the function <code>impute.pa</code> in the package <code>imp4p</code>

Value

The `exprs(obj)` matrix with imputed values instead of missing values.

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
dat <- mvFilter(Exp1_R25_pept[1:1000], type="allCond", th = 1)
dat <- wrapper.impute.pa(dat)
```

wrapper.impute.pa2 *Missing values imputation from a [MSnSet](#) object*

Description

This method is a wrapper to the function `impute.pa` from the package `imp4p` adapted to objects of class `MSnSet`.

Usage

```
wrapper.impute.pa2(obj, q.min = 0, q.norm = 3, eps = 0,  
  distribution = "unif")
```

Arguments

<code>obj</code>	An object of class <code>MSnSet</code> .
<code>q.min</code>	A quantile value of the observed values allowing defining the maximal value which can be generated. This maximal value is defined by the quantile <code>q.min</code> of the observed values distribution minus <code>eps</code> . Default is 0 (the maximal value is the minimum of observed values minus <code>eps</code>).
<code>q.norm</code>	A quantile value of a normal distribution allowing defining the minimal value which can be generated. Default is 3 (the minimal value is the maximal value minus $qn * \text{median}(\text{sd}(\text{observed values}))$ where <code>sd</code> is the standard deviation of a row in a condition).
<code>eps</code>	A value allowing defining the maximal value which can be generated. This maximal value is defined by the quantile <code>q.min</code> of the observed values distribution minus <code>eps</code> . Default is 0.
<code>distribution</code>	The type of distribution used. Values are <code>unif</code> or <code>beta</code> .

Value

The object `obj` which has been imputed

Author(s)

Thomas Burger, Samuel Wiczorek

Examples

```
require(DAPARdata)  
data(Exp1_R25_pept)  
wrapper.impute.pa2(Exp1_R25_pept[1:1000], distribution="beta")
```

wrapper.mvHisto	<i>Histogram of missing values from a MSnSet object</i>
-----------------	---

Description

This method plots from a [MSnSet](#) object a histogram of missing values.

Usage

```
wrapper.mvHisto(obj, indLegend = "auto", showValues = FALSE)
```

Arguments

obj	An object of class MSnSet .
indLegend	The indices of the column name's in <code>pData()</code> tab.
showValues	A logical that indicates wether numeric values should be drawn above the bars.

Value

A histogram

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.mvHisto(Exp1_R25_pept, showValues=TRUE)
```

wrapper.mvImage	<i>Heatmap of missing values from a MSnSet object</i>
-----------------	---

Description

Plots a heatmap of the quantitative data. Each column represent one of the conditions in the object of class [MSnSet](#) and the color is proportional to the mean of intensity for each line of the dataset. The lines have been sorted in order to vizualize easily the different number of missing values. A white square is plotted for missing values.

Usage

```
wrapper.mvImage(obj)
```

Arguments

obj	An object of class MSnSet .
-----	---

Value

A heatmap

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.mvImage(Exp1_R25_pept)
```

wrapper.mvImputation *Missing values imputation from a [MSnSet](#) object*

Description

This method is a wrapper to the `imputeLCMD` package adapted to objects of class [MSnSet](#).

Usage

```
wrapper.mvImputation(obj, method)
```

Arguments

obj	An object of class MSnSet .
method	The imputation method to be used. Choices are QRILC, KNN, BPCA and MLE.

Value

The object `obj` which has been imputed

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.mvImputation(Exp1_R25_pept[1:1000], "QRILC")
```

`wrapper.mvPerLinesHisto`*Histogram of missing values per lines from an object [MSnSet](#)*

Description

This method is a wrapper to plots from a [MSnSet](#) object a histogram which represents the distribution of the number of missing values (NA) per lines (ie proteins).

Usage

```
wrapper.mvPerLinesHisto(obj, indLegend = "auto", showValues = FALSE)
```

Arguments

<code>obj</code>	An object of class MSnSet .
<code>indLegend</code>	The indice of the column name's in <code>pData()</code> tab .
<code>showValues</code>	A logical that indicates wether numeric values should be drawn above the bars.

Value

A histogram

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.mvPerLinesHisto(Exp1_R25_pept)
```

`wrapper.mvPerLinesHistoPerCondition`*Bar plot of missing values per lines and per conditions from an object [MSnSet](#)*

Description

This method is a wrapper to plots from a [MSnSet](#) object a bar plot which represents the distribution of the number of missing values (NA) per lines (ie proteins) and per conditions.

Usage

```
wrapper.mvPerLinesHistoPerCondition(obj, indLegend = "auto",
  showValues = FALSE)
```

Arguments

obj	An object of class MSnSet .
indLegend	The indice of the column name's in pData() tab .
showValues	A logical that indicates wether numeric values should be drawn above the bars.

Value

A bar plot

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.mvPerLinesHistoPerCondition(Exp1_R25_pept)
```

wrapper.mvTypePlot	<i>Distribution of missing values with respect to intensity values from a MSnSet object</i>
--------------------	---

Description

This method plots a scatter plot which represents the distribution of missing values. The colors correspond to the different conditions (slot Label in in the dataset of class [MSnSet](#)). The x-axis represent the mean of intensity for one condition and one entity in the dataset (i. e. a protein) whereas the y-axis count the number of missing values for this entity and the considered condition. The data have been jittered for an easier vizualisation.

Usage

```
wrapper.mvTypePlot(obj, threshold = 0)
```

Arguments

obj	An object of class MSnSet .
threshold	An integer for the intensity that delimits MNAR and MCAR missing values.

Value

A scatter plot

Author(s)

Florence Combes, Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.mvTypePlot(Exp1_R25_pept)
```

 wrapper.normalizeD *Normalization*

Description

Provides several methods to normalize quantitative data from a [MSnSet](#) object. They are organized in four main families : Global Alignment, Median Centering, Mean Centering, Mean Centering Scaling. For the first family, two sub-categories are available : the sum by columns and the quantiles method. For the three other families, two categories are available : "Overall" which means that the value for each protein (ie line in the expression data tab) is computed over all the samples ; "within conditions" which means that the value for each protein (ie line in the exprs() data tab) is computed condition by condition.

Usage

```
wrapper.normalizeD(obj, family, method)
```

Arguments

obj	An object of class MSnSet .
family	One of the following : Global Alignment, Median Centering, Mean Centering, Mean Centering Scaling.
method	"overall" or "within conditions".

Value

An instance of class [MSnSet](#) where the quantitative data in the exprs() tab has been normalized.

Author(s)

Alexia Dorffer

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.normalizeD(Exp1_R25_pept[1:1000], "Median Centering", "within conditions")
```

 wrapper.normalizeD2 *Normalisation*

Description

Provides several methods to normalize quantitative data from a [MSnSet](#) object. They are organized in four main families : Strong Rescaling, Median Centering, Mean Centering, Mean Centering Scaling. For the first family, two sub-categories are available : the sum by columns and the quantiles method. For the three other families, two categories are available : "Overall" which means that the value for each protein (ie line in the expression data tab) is computed over all the samples ; "within conditions" which means that the value for each protein (ie line in the exprs() data tab) is computed condition by condition.

Usage

```
wrapper.normalizedD2(obj, method, type, scaling = FALSE, quantile = 0.15)
```

Arguments

obj	An object of class MSnSet .
method	One of the following : Global Alignment (for normalizations of important magnitude), Quantile Centering, Mean Centering.
type	For the method "Global Alignment", the parameters are: "sum by columns": operates on the original scale (not the log2 one) and propose to normalize each abundance by the total abundance of the sample (so as to focus on the analyte proportions among each sample). "Alignment on all quantiles": proposes to align the quantiles of all the replicates; practically it amounts to replace abundances by order statistics. For the two other methods, the parameters are "overall" (shift all the sample distributions at once) or "within conditions" (shift the sample distributions within each condition at a time).
scaling	A boolean that indicates if the variance of the data have to be forced to unit (variance reduction) or not.
quantile	A float that corresponds to the quantile used to align the data.

Value

An instance of class [MSnSet](#) where the quantitative data in the `exprs()` tab has been normalized.

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
wrapper.normalizedD2(Exp1_R25_pept[1:1000], "Quantile Centering", "within conditions")
```

`wrapper.violinPlotD` *Wrapper to the `violinPlotD` function on an object [MSnSet](#)*

Description

This function is a wrapper for using the `violinPlotD` function with objects of class [MSnSet](#)

Usage

```
wrapper.violinPlotD(obj, dataForXAxis = "Label", group2Color = "Condition")
```

Arguments

obj	An object of class MSnSet .
dataForXAxis	A vector of strings containing the names of columns in <code>pData()</code> to print labels on X-axis (Default is "Label").
group2Color	A string that indicates how to color the replicates: one color per condition (value "Condition") or one color per replicate (value "Replicate"). Default value is by Condition.

Value

A violin plot

Author(s)

Samuel Wieczorek

See Also

[wrapper.densityPlotD](#), [wrapper.boxPlotD](#)

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
library(vioplot)
types <- c("Label", "Analyt.Rep")
wrapper.violinPlotD(Exp1_R25_pept, types)
```

wrapperCalibrationPlot

Performs a calibration plot on an [MSnSet](#) object, calling the `cp4p` package functions.

Description

This function is a wrapper to the `calibration.plot` method of the `cp4p` package for use with [MSnSet](#) objects.

Usage

```
wrapperCalibrationPlot(vPVal, pi0Method = "pounds")
```

Arguments

vPVal	A dataframe that contains quantitative data.
pi0Method	A vector of the conditions (labels) (one label per sample).

Value

A plot

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R25_pept)
condition1 <- '25fmol'
condition2 <- '10fmol'
qData <- Biobase::exprs(Exp1_R25_pept[1:1000])
labels <- Biobase::pData(Exp1_R25_pept[1:1000])[,"Label"]
diffAnaWelch(qData, labels, condition1, condition2)
```

writeMSnsetToExcel *This function exports a [MSnSet](#) object to a Excel file.*

Description

This function exports a [MSnSet](#) data object to a Excel file. Each of the three data.frames in the [MSnSet](#) object (ie experimental data, phenoData and metaData are respectively integrated into separate sheets in the Excel file).

Usage

```
writeMSnsetToExcel(obj, filename)
```

Arguments

obj An object of class [MSnSet](#).
filename A character string for the name of the Excel file.

Value

A Excel file (.xlsx)

Author(s)

Samuel Wieczorek

Examples

```
require(DAPARdata)
data(Exp1_R2_pept)
obj <- Exp1_R2_pept[1:1000]
writeMSnsetToExcel(obj, "foo")
```

Index

boxPlotD, [3](#), [11](#)
BuildAdjacencyMatrix, [4](#)
BuildColumnToProteinDataset, [5](#)

compareNormalizationD, [6](#)
corrMatrixD, [7](#)
CountPep, [7](#)
createMSnset, [8](#)
CVDistD, [9](#), [11](#)

deleteLinesFromIndices, [10](#)
densityPlotD, [3](#), [9](#), [10](#), [44](#)
diffAna, [11](#), [12](#), [15](#)
diffAnaComputeFDR, [12](#)
diffAnaGetSignificant, [13](#)
diffAnaLimma, [14](#)
diffAnaSave, [15](#)
diffAnaVolcanoplot, [16](#)
diffAnaVolcanoplot_rCharts, [17](#)
diffAnaWelch, [18](#)

getIndicesConditions, [19](#)
getIndicesOfLinesToRemove, [20](#)
getNumberOf, [20](#)
getNumberOfEmptyLines, [21](#)
getPaletteForLabels, [22](#)
getPaletteForReplicates, [22](#)
getPourcentageOfMV, [23](#)
getProcessingInfo, [24](#)
getProteinsStats, [24](#)
GraphPepProt, [25](#)

heatmap.2, [26](#), [27](#), [50](#)
heatmap.DAPAR, [26](#)
heatmapD, [27](#)

impute.pa2, [27](#)

limma, [11](#), [15](#)
limmaCompleteTest, [28](#)

MeanPeptides, [29](#)
MSnbase, [4](#), [24](#), [39](#)
MSnSet, [7](#), [8](#), [10](#), [11](#), [13–15](#), [18](#), [20](#), [23](#), [26–28](#),
[30–33](#), [36](#), [40](#), [44](#), [46–60](#)

mvFilter, [30](#)
mvFilterFromIndices, [31](#)
mvFilterGetIndices, [32](#)
mvHisto, [33](#)
mvImage, [33](#)
mvImputation, [34](#)
mvPerLinesHisto, [35](#)
mvPerLinesHistoPerCondition, [35](#)
mvTypePlot, [36](#)

normalized, [37](#)
normalized2, [38](#)

pepAgregate, [39](#)
proportionConRev, [39](#)

RColorBrewer, [22](#)
removeLines, [40](#)

SumPeptides, [41](#)

t.test, [18](#), [50](#)
TopnPeptides, [42](#)
translatedRandomBeta, [42](#)

violinPlotD, [43](#)

wrapper.boxPlotD, [44](#), [49](#), [59](#)
wrapper.compareNormalizationD, [45](#)
wrapper.corrMatrixD, [46](#)
wrapper.CVDistD, [46](#), [49](#)
wrapper.dapar.impute.mi, [47](#)
wrapper.densityPlotD, [44](#), [47](#), [48](#), [59](#)
wrapper.diffAnaLimma, [49](#)
wrapper.diffAnaWelch, [50](#)
wrapper.heatmapD, [50](#)
wrapper.impute.pa, [51](#)
wrapper.impute.pa2, [52](#)
wrapper.mvHisto, [53](#)
wrapper.mvImage, [53](#)
wrapper.mvImputation, [54](#)
wrapper.mvPerLinesHisto, [55](#)
wrapper.mvPerLinesHistoPerCondition,
[55](#)
wrapper.mvTypePlot, [56](#)

`wrapper.normalized`, [57](#)
`wrapper.normalized2`, [57](#)
`wrapper.violinPlotD`, [58](#)
`wrapperCalibrationPlot`, [59](#)
`writeMSnsetToExcel`, [60](#)