Package 'SafeQuant'

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Type Package

Title A Toolbox for the Analysis of Proteomics Data

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Author Erik Ahrne

Maintainer Erik Ahrne <erik.ahrne@unibas.ch>

Description Tools for the statistical analysis and visualization of (relative
and absolute) quantitative (LFQ,TMT,HRM) Proteomics data.

Imports limma,
gplots,
seqinr,
corrplot,
optparse,
data.table,
epiR,
Biobase,

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RoxygenNote 5.0.1

R topics documented:

addIdQvalues   *Add identification leve q-values to ExpressionSet (calculated based on target-decoy score distribution)*

Description

Add identification leve q-values to ExpressionSet (calculated based on target-decoy score distribution)

Usage

```
addIdQvalues(eset = eset)
```

Arguments

eset   ExpressionSet

Details

if ptm column is part if the ExpressionSet q-values are calculated seperately for modified and non-modified features

No details

Value

ExpressionSet object

Note

No note

See Also

getIdLevelQvals

Examples

```
print("No examples")
```

---

addScaffoldPTMFAnnotations

Add scaffold ptm annotaitons to tmt experiment

Description

Add scaffold ptm annotaitons to tmt experiment

Usage

```
addScaffoldPTMFAnnotations(eset, file)
```

Arguments

eset   ExpressionSet

file   path to Scaffold file

Value

ExpressionSet object

Note

No note

References

No references

Examples

```
print("No examples")
```

---

barplotMSSignal   *Barplot of ms-signal per column*

Description

Barplot of ms-signal per column

Usage

```
barplotMSSignal(eset,
  col = as.character(.getConditionColors(eset)[pData(eset)$condition, ]),
  method = c("sum", "sharedSignal"), cex.lab = 1.25, cex.axis = 1.25,
  cex.names = 0.9, labels = rownames(pData(eset)), ...)
```

Arguments

`eset`	expressionSet
`col`	default condition colors
`method`	c("median","sum","sharedSignal")
`cex.lab`	default 1.25
`cex.axis`	default 1.25
`cex.names`	default 0.9
`labels`	labels
`...`	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

COLORS	*color vector*

Description

color vector

Usage

```
COLORS
```

Format

An object of class `character` of length 668.

---

createExpDesign   *Create Experimental Design*

Description

Create Experimental Design

Usage

```
createExpDesign(tag, nbPlex)
```

Arguments

tag   user input tag e.g. 1,2,3:4,5,6 indicating two condition with 3 reps each

nbPlex   tmt 6 or 10 plex

Details

The first listed condition is always the control condition

No details

Value

expDesign data.frame

Note

No note

References

NA

Examples

```
print("No examples")
```

---

createExpressionDataset
                              Create ExpressionSet object

Description

Create ExpressionSet object

Usage

```
createExpressionDataset(expressionMatrix = expressionMatrix,
  expDesign = expDesign, featureAnnotations = featureAnnotations)
```

Arguments

expressionMatrix

         matrix of expression signals per feature and sample

expDesign   experimental design data.frame

featureAnnotations

         data.frame including e.g: Protein Description, Id score etc.

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

[ExpressionSet]

Examples

```
print("No examples")
```

---

createPairedExpDesign   *Create Paired Expdesign*

Description

Create Paired Expdesign

Usage

```
createPairedExpDesign(eset)
```

Arguments

eset   ExpressionSet

Details

Add subject colum to phenoData design data.frame

Value

ExpressionSet object

Note

No note

References

NA

See Also

[ExpressionSet](#)

Examples

```
print("No examples")
```

---

cvBoxplot   *C.V. boxplot*

Description

C.V. boxplot

Usage

```
cvBoxplot(eset,
  col = as.character(.getConditionColors(eset)[unique(pData(eset)$condition),
  ]), cex.names = 0.9, cex.axis = 1.25, cex.lab = 1.25,
  ylab = "C.V. (%)", ...)
```

Arguments

eset	ExpressionSet
col	col
cex.names	default 0.9
cex.axis	default 1.25
cex.lab	default 1.25
ylab	C.V.
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

```
expDesignTagToExpDesign
```
Create experimental design data.frame from user input string

Description

Create experimental design data.frame from user input string

Usage

```
expDesignTagToExpDesign(tag, expDesignDefault)
```

Arguments

```
tag               tag
expDesignDefault
                  data.frame
```

Details

tag: 1,2:3:4,5,6 condition isControl 1 Condition 1 TRUE 2 Condition 1 TRUE 3 Condition 1 TRUE 4 Condition 2 FALSE 5 Condition 2 FALSE 6 Condition 2 FALSE

Value

data.frame describing experimental design

Note

No note

References

NA

Examples

```
print("No examples")
```

---

export   *Export content of safeQuantAnalysis object*

Description

Export content of safeQuantAnalysis object

Usage

```
export(sqa, nbRows = nrow(sqa$pValue), file = NA)
```

Arguments

sqa	safeQuantAnalysis object
nbRows	Number of rows to export. Features are ordred by increasing minimal p.value
file	file path

Details

NA

Note

No note

References

NA

See Also

safeQuantAnalysis

Examples

```
print("No examples")
```

---

getAAProteinCoordinates
                          Get amino acid coordinates on protein

---

Description

Get amino acid coordinates on protein

Usage

```
getAAProteinCoordinates(peptideSeq, proteinSeq, aaRegExpr = "[STY]")
```

Arguments

`peptideSeq`	peptide sequence
`proteinSeq`	protein sequence
`aaRegExpr`	target AA reg exp

Details

NA

Value

vector of protein coordinates (mmodification residue number)

Note

No note

References

NA

Examples

```
print("No examples")
```

`getAllCV`	*Calculate Coefficiant of Variance per feature (Relative standard Deviation) per Condition*

Description

Calculate Coefficiant of Variance per feature (Relative standard Deviation) per Condition

Usage

```
getAllCV(eset)
```

Arguments

`eset`	ExpressionSet

Details

CV = sd / mean

Value

data.frame of CVs per condition

Note

No note

References

NA

See Also

getCV

Examples

```
print("No examples")
```

---

getAllEBayes   *Perform statistical test (mderated t-test), comparing all case to control*

Description

Perform statistical test (mderated t-test), comparing all case to control

Usage

```
getAllEBayes(eset = eset, adjust = F, log = T, method = "pairwise",
  adjustFilter = matrix(F, nrow = nrow(eset), ncol =
  length(levels(pData(eset)$condition)) - 1))
```

Arguments

eset	ExpressionSet
adjust	TRUE/FALSE adjust for multiple testing using Benjamini & Hochberg (1995) method
log	T/F log-transform expression values
method	c("all","pairwise")
adjustFilter	matrix T/F do not adjust for multiple testing

Details

No details

Value

ExpressionSet object

Note

No note

References

Empirical Bayes method, Smyth (2004), <http://www.ncbi.nlm.nih.gov/pubmed/16646809>

See Also

eBayes

Examples

```
print("No examples")
```

---

getBaselineIntensity	*Get signal at zscore x (x standard deviations below mean)*

Description

Get signal at zscore x (x standard deviations below mean)

Usage

```
getBaselineIntensity(intensities, promille = 5)
```

Arguments

intensities	refrence run signals
promille	baseline value set as specified promille

Value

baseline value

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getCV	*Calculate Coefficiant of Variance per feature (Relative standard Deviation)*

Description

Calculate Coefficiant of Variance per feature (Relative standard Deviation)

Usage

```
getCV(data)
```

Arguments

data	data.frame of replicate signals

Details

CV = sd / mean

Value

vector of CVs

Note

No note

References

NA

Examples

```
print("No examples")
```

```
getExpDesignProgenesisCsv
```

Parse Experimental Design from Progenesis Csv Export

Description

Parse Experimental Design from Progenesis Csv Export

Usage

```
getExpDesignProgenesisCsv(file,
  expressionColIndices = .getProgenesisCsvExpressionColIndices(file))
```

Arguments

```
file              path to progenesis csv file
expressionColIndices
                  default .getProgenesisCsvExpressionColIndices(file)
```

Details

No details

Value

data.frame describing experimental design

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getGlobalNormFactors	*Get normalization factors. calculated as summed/median signal per run (column) over summed/median of first run.*

Description

Get normalization factors. calculated as summed/median signal per run (column) over summed/median of first run.

Usage

```
getGlobalNormFactors(eset, method = "median")
```

Arguments

eset   ExpressionSet

method   c("sum","median)

Details

No details

Value

vector of normalization factors

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getIBAQEset   *Calculate intensity-based absolute-protein-quantification (iBAQ) metric per protein*

Description

Calculate intensity-based absolute-protein-quantification (iBAQ) metric per protein

Usage

```
getIBAQEset(eset, proteinDB = NA, peptideLength = c(5, 36),
  nbMiscleavages = 0, proteaseRegExp = .getProteaseRegExp("trypsin"))
```

Arguments

eset	protein level ExpressionSet
proteinDB	list protein sequneces
peptideLength	peptide length interval (to get number of peptides used for normalization)
nbMiscleavages	number of mis-cleavages allowed when digesting protein sequneces in silico (to get number of peptides used for normalization)
proteaseRegExp	protease Reg Exp cleavage rule

Details

No details

Value

ExpressionSet

Note

No note

References

Global quantification of mammalian gene expression control, Schwanhausser (2011), http://www.ncbi.nlm.nih.gov/pubmed/21593866, Critical assessment of proteome-wide label-free absolute abundance estimation strategies. Ahrne (2013), http://www.ncbi.nlm.nih.gov/pubmed/23794183

Examples

```
print("No examples")
```

getIdLevelQvals	*Calculates identification level q-values based on target-decoy score distributions*

Description

Calculates identification level q-values based on target-decoy score distributions

Usage

```
getIdLevelQvals(scores, isDecoy)
```

Arguments

scores   peptide/protein identficationscore

isDecoy   vector of TRUE/FALSE

Details

q-value = (Nb. Decoy Entries at idScore Threshold S*) / (Nb. Target Entries at idScore Threshold S). (* idScore >= S)

Value

vector of q.values

Note

No note

References

NA

Examples

```
print("No examples")
```

getImpuritiesMatrix	*Get Thermo TMT impurity matrix*

Description

Get Thermo TMT impurity matrix

Usage

```
getImpuritiesMatrix(plexNb = 6)
```

Arguments

plexNb   integer, 6 or 10 plex

Details

No details

Value

impurity matrix matrix

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getIntSumPerProtein   *Sum up raw intensities per protein and channel. keep track of number of summed spectra and unique peptides*

Description

Sum up raw intensities per protein and channel. keep track of number of summed spectra and unique peptides

Usage

```
getIntSumPerProtein(intData, proteinACs, peptides, minNbPeptPerProt = 1)
```

Arguments

intData   data.frame of intensities per channel

proteinACs   vector of protein accession numbers

peptides   vector of peptide sequneces

minNbPeptPerProt
                        minimal number of peptides per protein

Details

NA

No details

Value

list containing 3 objects 1) data.frame of channel intensities per protein ac, 2) vector listing number of summed spectra per protein, 3) vector listing number of summed peptides per protein

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getLoocvFoldError   *Leave-One-Out Cross Validate Qunatification Model*

Description

Leave-One-Out Cross Validate Qunatification Model

Usage

```
getLoocvFoldError(df)
```

Arguments

df   data.frame of two columns 1) "signal" - ms metric 2) "cpc" absolute quantity

Details

No details

Value

data.frame of fold errors per (left-out) protein

Note

No note

References

NA

See Also

NA

Examples

```
print("No examples")
```

---

getMaxIndex *get index of max in vecotr of numeric values*

Description

get index of max in vecotr of numeric values

Usage

```
getMaxIndex(v)
```

Arguments

v   vector

---

getMeanCenteredRange *Get modification coordinates on protein*

Description

Get modification coordinates on protein

Usage

```
getMeanCenteredRange(d, nbSd = 4)
```

Arguments

d   numeric vector

nbSd   range spanning number of sd frmo mean

Details

NA

Value

vector range boundries

Note

No note

References

NA

Examples

```
print("No examples")
```

getModifProteinCoordinates

Get modification coordinates on protein

Description

Get modification coordinates on protein

Usage

```
getModifProteinCoordinates(modifAnnot, peptideSeq, proteinSeq, format = 1)
```

Arguments

modifAnnot	modifcation as annotated by progenesis. E.g. '[15] Phospho (ST)|[30] Phospho (ST)'
peptideSeq	peptide sequence
proteinSeq	protein sequence
format	c(1,2) 1. progenesis 2. scaffold

Details

NA

Value

vector of protein coordinates (mmodification residue number)

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getMotifX   *Create motif-x peptide annotation*

Description

Create motif-x peptide annotation

Usage

```
getMotifX(modifPos, peptide, proteinSeq, motifLength = 4)
```

Arguments

modifPos	vector positions
peptide	peptide sequence
proteinSeq	protein sequence
motifLength	motif flanking sequence

Details

motif-x example PGDYS*TTPG

Value

vector of motifs

Note

No note

References

NA

Examples

```
print("No examples")
```

getNbDetectablePeptides

Get number peptides passing defined length criteria

Description

Get number peptides passing defined length criteria

Usage

```
getNbDetectablePeptides(peptides, peptideLength = c(5, 36))
```

Arguments

peptides   list of peptides

peptideLength   vector of two integers defining peptide length range

Details

No details

Value

integer corresponding to number of detectable peptides

Note

No note

Examples

```
print("No examples")
```

getNbMisCleavages   *Get number of mis-cleavages perp peptide*

Description

Get number of mis-cleavages perp peptide

Usage

```
getNbMisCleavages(peptide, protease = "trypsin")
```

Arguments

peptide   character vector

protease   regular expression

Details

NA

Value

vector ofintegers

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getNbPeptidesPerProtein

Get number of peptides per protein

Description

Get number of peptides per protein

Usage

```
getNbPeptidesPerProtein(eset)
```

Arguments

eset   ExpressionSet

Details

NA

Value

table

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getNbSpectraPerProtein
Get number of spectra per protein

Description

Get number of spectra per protein

Usage

```
getNbSpectraPerProtein(eset)
```

Arguments

eset   ExpressionSet

Details

NA

Value

table

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getPeptides   *Digest protein*

Description

Digest protein

Usage

```
getPeptides(proteinSeq, proteaseRegExp = .getProteaseRegExp("trypsin"),
  nbMiscleavages = 0)
```

Arguments

`proteinSeq`	protein sequence
`proteaseRegExp`	protease Regular Expression
`nbMiscleavages`	default 0

Details

No details

Value

vector of peptides

Note

No note

Examples

```
print("No examples")
```

`getRatios`	*Calculate ratios, comparing all case to control*

Description

Calculate ratios, comparing all case to control

Usage

```
getRatios(eset, method = "median", log2 = T)
```

Arguments

`eset`	ExpressionSet
`method`	median, mean, paired
`log2`	transform

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getRTNormFactors *Get retentiontime base normalization factors*

Description

Get retentiontime base normalization factors

Usage

```
getRTNormFactors(eset, minFeaturesPerBin = 100)
```

Arguments

eset   ExpressionSet

minFeaturesPerBin

                minumum number of features per bin. If nb. features are < minFeaturesPerBin
                -> include neighbouring bins.

Details

No details

Value

data.frame normalization factors per retention time bin (minute)

Note

No note

References

In Silico Instrumental Response Correction Improves Precision of Label-free Proteomics and Accuracy of Proteomics-based Predictive Models, Lyutvinskiy et al. (2013), http://www.ncbi.nlm.nih.gov/pubmed/23589346

Examples

```
print("No examples")
```

---

getScoreCutOff   *Get score cutoff for a given fdr cut-off*

Description

Get score cutoff for a given fdr cut-off

Usage

```
getScoreCutOff(scores, isDecoy, fdrCutOff = 0.01)
```

Arguments

scores	peptide/protein identficationscore
isDecoy	vector of TRUE/FALSE
fdrCutOff	[0,1]

Details

NA

Value

scoreCutoff

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getSignalPerCondition   *Summarize replicate signal per condition (min)*

Description

Summarize replicate signal per condition (min)

Usage

```
getSignalPerCondition(eset, method = "median")
```

Arguments

eset	ExpressionSet
method	median (default), mean, max, min, sd

Details

No details

Value

data.frame of per condition signals

Note

No note

References

NA

Examples

```
print("No examples")
```

---

getTopX	*Calculate Mean of X most intense features*

Description

Calculate Mean of X most intense features

Usage

```
getTopX(entryData, topX = 3)
```

Arguments

entryData	data.frame listing feature intensities of one entry. Typically rows corresponds to Peptide entries of one protein
topX	best X flyers

Details

No details

Value

vector of topX intensities per column (sample)

Note

No note

References

Absolute quantification of proteins by LCMSE: A virtue of parallel MS acquisition, Silva (2006), <http://www.ncbi.nlm.nih.gov/pubmed/16219938>, Critical assessment of proteome-wide label-free absolute abundance estimation strategies. Ahrne (2013), <http://www.ncbi.nlm.nih.gov/pubmed/23794183>

Examples

```
print("No examples")
```

---

getUserOptions	*Read User Specified Command Line Options*

Description

Read User Specified Command Line Options

Usage

```
getUserOptions(version = version)
```

Arguments

version   Safequant version number

Details

No details

Value

user options list

Note

No note

References

NA

Examples

```
print("No examples")
```

---

globalNormalize	*Normalize, Norm factors calculated as median signal per run (column) over median of first run.*

Description

Normalize, Norm factors calculated as median signal per run (column) over median of first run.

Usage

```
globalNormalize(eset, globalNormFactors)
```

Arguments

eset   ExpressionSet

globalNormFactors

globalNormFactors

Details

No details

Value

eset ExpressionSet

Note

No note

References

NA

See Also

getGlobalNormFactors

Examples

```
print("No examples")
```

hClustHeatMap   *Hierarchical clustering heat map, cluster by runs intensity, features by ratio and display log2 ratios to control median*

Description

Hierarchical clustering heat map, cluster by runs intensity, features by ratio and display log2 ratios to control median

Usage

```
hClustHeatMap(eset, conditionColors = .getConditionColors(eset),
  breaks = seq(-2, 2, length = 20), dendogram = "column",
  legendPos = "left", ...)
```

Arguments

eset   ExpressionSet

conditionColors
                  data.frame of colors per condition

breaks   default seq(-2,2,length=20)

dendogram   see heatmap.2 gplots

legendPos   see legend

...   see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

isCon   *Check if protein is a contaminant entry*

Description

Check if protein is a contaminant entry

Usage

```
isCon(ac)
```

Arguments

ac   vector of protein accession numbers

Details

contanminants proteins are typically annotated as: CON_P0000

Value

vector TRUE/FALSE

Note

No note

References

NA

Examples

```
print("No examples")
```

---

isDecoy   *Check if protein is a decoy entry*

Description

Check if protein is a decoy entry

Usage

```
isDecoy(ac)
```

Arguments

ac   vector of protein accession numbers

Details

decoy proteins are typically annotated as: REV_P0000

Value

vector TRUE/FALSE

Note

No note

References

NA

Examples

```
print("No examples")
```

---

isStrippedACs	*Check if ACs are in "non-stripped" uniprot format e.g. "sp|Q8CHJ2|AQP12_MOUSE"*

Description

Check if ACs are in "non-stripped" uniprot format e.g. "sp|Q8CHJ2|AQP12_MOUSE"

Usage

```
isStrippedACs(acs)
```

Arguments

acs   accession numbers

Details

TRUE if less than 10

Value

boolean TRUE/FALSE

Note

No note

References

NA

Examples

```
print("No examples")
```

---

maPlotSQ   *ma-plot*

Description

ma-plot

Usage

```
maPlotSQ(eset, sample = colnames(exprs(eset))[1], cex.lab = 1.5,
  cex.axis = 1.5, lwd = 2, pch = 1, col = rgb(0, 100, 0, 50,
  maxColorValue = 255), ...)
```

Arguments

eset	ExpressionSet
sample	selected condition
cex.lab	default 1.5
cex.axis	default 1.5
lwd	default 2
pch	default 1
col	green transparent
...	see plot

Note

No note

References

NA

Examples

```
print("No examples")
```

---

missinValueBarplot   *Plot Percentage of Features with with missing values*

Description

Plot Percentage of Features with with missing values

Usage

```
missinValueBarplot(eset,
  col = as.character(.getConditionColors(eset)[pData(eset)$condition, ]),
  cex.axis = 1.25, cex.lab = 1.25, ...)
```

Arguments

`eset`	ExpressionSet
`col`	col
`cex.axis`	cex.axis
`cex.lab`	cex.lab
`...`	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

`option_list` *Command Line Option List*

Description

Command Line Option List

Usage

```
option_list
```

Format

An object of class list of length 29.

pairsAnnot	*Plot lower triangle Pearsons R^2. Diagonal text, upper triangle all against all scatter plots with lm abline*

Description

Plot lower triangle Pearsons R^2. Diagonal text, upper triangle all against all scatter plots with lm abline

Usage

```
pairsAnnot(data, textCol = rep(1, ncol(data)), diagText = colnames(data),
  col = rgb(0, 100, 0, 50, maxColorValue = 255), isHeatCol = F,
  cexTxt = 2, ...)
```

Arguments

data	data.frame
textCol	text color
diagText	diagnoal text
col	dot col
isHeatCol	heat colors
cexTxt	cex txt
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

parseMaxQuantProteinGroupTxt

Parse MaxQuant Protein Group Txt

Description

Parse MaxQuant Protein Group Txt

Usage

```
parseMaxQuantProteinGroupTxt(file = file, expDesign = expDesign,
  method = "auc")
```

Arguments

file	path to MaxQuant Protein txt file
expDesign	experimental design data.frame
method	auc (area under curve) or spc (spectral count)

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

ExpressionSet

Examples

```
print("No examples")
```

parseProgenesisFeatureCsv

Parse Progenesis Feature Csv Export

Description

Parse Progenesis Feature Csv Export

Usage

```
parseProgenesisFeatureCsv(file = file,
  expDesign = getExpDesignProgenesisCsv(file), method = "auc")
```

Arguments

file	path to Progenesis Feature csv file
expDesign	experimental design data.frame
method	auc (area under curve) or spc (spectral count)

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

[ExpressionSet]

Examples

```
print("No examples")
```

parseProgenesisPeptideMeasurementCsv

Parse Progenesis Peptide Measurement Csv Export

Description

Parse Progenesis Peptide Measurement Csv Export

Usage

```
parseProgenesisPeptideMeasurementCsv(file, expDesign = expDesign,
  method = "auc",
  expressionColIndices = .getProgenesisCsvExpressionColIndices(file, method =
  method), uniqueProteins = F)
```

Arguments

file	path to Progenesis Peptide Measurement csv file
expDesign	experimental design data.frame
method	auc (area under curve) or spc (spectral count)
expressionColIndices	
	default .getProgenesisCsvExpressionColIndices()
uniqueProteins	T/F keep unique peptides only

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

[ExpressionSet](#)

Examples

```
print("No examples")
```

parseProgenesisProteinCsv

Parse Progenesis Protein Csv

Description

Parse Progenesis Protein Csv

Usage

```
parseProgenesisProteinCsv(file = file, expDesign = expDesign,
  method = "auc")
```

Arguments

file	path to Progenesis Protein csv file
expDesign	experimental design data.frame
method	auc (area under curve) or spc (spectral count)

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

[ExpressionSet]

Examples

```
print("No examples")
```

parseScaffoldPTMReport
Parse scaffold PTM Spectrum Report

Description

Parse scaffold PTM Spectrum Report

Usage

```
parseScaffoldPTMReport(file)
```

Arguments

file   path to Scaffold file

Details

No details

Value

data.frame

Note

No note

References

NA

Examples

```
print("No examples")
```

parseScaffoldRawFile   *Parse scaffold output .xls file (RAW export)*

Description

Parse scaffold output .xls file (RAW export)

Usage

```
parseScaffoldRawFile(file, expDesign = expDesign, keepFirstAcOnly = FALSE,
  isPurityCorrect = T)
```

Arguments

file   path to Scaffold file

expDesign   experimental design data.frame

keepFirstAcOnly

      TRUE/FALSE If multiple ACs in Accession.Numbers filed. Then keep the first one only

isPurityCorrect

      do purity correction

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

ExpressionSet

Examples

```
print("No examples")
```

---

perFeatureNormalization

Per Feature Normalization

Description

Per Feature Normalization

Usage

```
perFeatureNormalization(eset, normFactors)
```

Arguments

eset   ExpressionSet

normFactors matrix normalization factors (logged) (row names are proteins)

Details

Example Usage: Normalize phospho peptide signals for Protein Changes

Value

ExpressionSet object

Note

No note

References

No references

Examples

```
print("No examples")
```

plotAbsEstCalibrationCurve

Plot absolut Estimation calibration Curve

Description

Plot absolut Estimation calibration Curve

Usage

```
plotAbsEstCalibrationCurve(fit, dispElements = c("formula", "lowess",
  "stats"), xlab = "Conc. (CPC) ", ylab = "Pred. Conc. (CPC) ",
  predictorName = paste("log10(", names(coef(fit))[2], ")", sep = ""),
  text = F, cex.lab = 1, cex.axis = 1, cex.text = 1, cex.dot = 1,
  main = "", ...)
```

Arguments

fit	simple log-linear model
dispElements	c("formula","lowess","stats")
xlab	xlab
ylab	ylab
predictorName	predictorName
text	add names beside each dot
cex.lab	expansion factor for axis labels
cex.axis	expansion factor for axis
cex.text	expansion factor for legend
cex.dot	expansion factor for plotted dots
main	main
...	see plot

Note

No note

References

NA

Examples

```
print("No examples")
```

```
plotAdjustedVsNonAdjustedRatio
```
Plot adjusted tmt ratios vs original ratios

Description

Plot adjusted tmt ratios vs original ratios

Usage

```
plotAdjustedVsNonAdjustedRatio(ratio, unAdjustedRatio)
```

Arguments

ratio   data.frame
unAdjustedRatio
                data.frame

Details

plot adjusted tmt ratios vs original ratios

Note

No note

References

NA

Examples

```
print("No examples")
```

---

plotExpDesign   *Display experimental design, high-lighting the control condition*

Description

Display experimental design, high-lighting the control condition

Usage

```
plotExpDesign(eset, condColors = .getConditionColors(eset), version = "X")
```

Arguments

eset	ExpressionSet
condColors	condition colors
version	version number

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

plotIdScoreVsFDR   *Plot FDR vs. identification score*

Description

Plot FDR vs. identification score

Usage

```
plotIdScoreVsFDR(idScore, qvals, qvalueThrs = 0.01,
  ylab = "False Discovery Rate", xlab = "Identification Score", ...)
```

Arguments

idScore	vector of identification scores
qvals	vector of q-valres
qvalueThrs	threshold indicated by horizontal line
ylab	default False Discovery Rate
xlab	default Identification Score
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

plotMSSignalDistributions

Plot ms.signal distributions

Description

Plot ms.signal distributions

Usage

```
plotMSSignalDistributions(d, col = 1:100, ylab = "Frequnecy",
  xlab = "MS-Signal", ...)
```

Arguments

d	matrix of ms-signals
col	color
ylab	default "Frequnecy"
xlab	default "MS-Signal"
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

plotNbIdentificationsVsRT

Plot the number of identified Features per Reteintion Time minute.

Description

Plot the number of identified Features per Reteintion Time minute.

Usage

```
plotNbIdentificationsVsRT(eset, cex.axis = 1.25, cex.lab = 1.25,
  col = "blue", lwd = 2, ...)
```

Arguments

eset	ExpressionSet
cex.axis	default 1.25
cex.lab	default 1.25
col	default "blue"
lwd	default 2
...	see plot see plot

Note

No note

References

NA

Examples

```
print("No examples")
```

```
plotNbValidDeFeaturesPerFDR
```
Plot Total Number of diffrentially Abundant Features (applying ratio cutoff) vs. qValue/pValue for all conditions

Description

Plot Total Number of diffrentially Abundant Features (applying ratio cutoff) vs. qValue/pValue for all conditions

Usage

```
plotNbValidDeFeaturesPerFDR(sqa, upRegulated = T, log2RatioCufOff = log2(1),
  pvalCutOff = 1, isLegend = T, isAdjusted = T, ylab = "Nb. Features",
  xlim = NA, ylim = NA, ...)
```

Arguments

sqa	SafeQuantAnalysis Object
upRegulated	TRUE/FALSE select for upregulated features
log2RatioCufOff	
	log2 ratio cut-off
pvalCutOff	pValue/qValue cut-off
isLegend	TRUE/FALSE display legend
isAdjusted	TRUE/FALSE qValues/pValue on x-axis
ylab	default Nb. Features
xlim	see plot
ylim	see plot
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

`plotPrecMassErrorDistrib`
Plot Precursor Mass Error Distribution

Description

Plot Precursor Mass Error Distribution

Usage

```
plotPrecMassErrorDistrib(eset, pMassTolWindow = c(-10, 10), ...)
```

Arguments

eset	ExpressionSet
pMassTolWindow	Precursor Mass Error Tolerance Window
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

`plotPrecMassErrorVsScore`
Plot precursorMass error v.s score highlighting decoy and displaying user specified user specified precursor mass filter

---

Description

Plot precursorMass error v.s score highlighting decoy and displaying user specified user specified precursor mass filter

Usage

```
plotPrecMassErrorVsScore(eset, pMassTolWindow = c(-10, 10), ...)
```

Arguments

`eset`	ExpressionSet
`pMassTolWindow`	Precursor Mass Error Tolerance Window
`...`	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

`plotQValueVsPValue`	*Plot qValue vs pValue*

Description

Plot qValue vs pValue

Usage

```
plotQValueVsPValue(sqa, lim = c(0, 1), ...)
```

Arguments

`sqa`	SafeQuantAnalysis Object
`lim`	x-axis and y-axis range
`...`	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

plotROC

Plot Number of Identifications vs. FDR

Description

Plot Number of Identifications vs. FDR

Usage

```
plotROC(qvals, qvalueThrs = 0.01, xlab = "False Discovery Rate",
  ylab = "Nb. Valid Identifications", xlim = c(0, 0.1), breaks = 100,
  col = "blue", lwd = 1.5, ...)
```

Arguments

qvals	vector of q-values
qvalueThrs	threshold indicated by vertical line
xlab	default "False Discovery Rate"
ylab	default "Nb. Valid Identifications"
xlim	default c(0,0.1)
breaks	see breaks for hist function
col	default blue
lwd	default 1.5
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

plotRTNorm *Plot all retention time profile overalying ratios*

Description

Plot all retention time profile overalying ratios

Usage

```
plotRTNorm(rtNormFactors, eset, samples = 1:ncol(rtNormFactors), main = "",
  ...)
```

Arguments

rtNormFactors	data.frame of normalization factor per r.t bin and sample, obtained by getRT-NormFactors
eset	ExprsssionSet
samples	specify samples (sample numbers) to be plotted
main	main
...	see plot see plot

Details

No details

Note

No note

References

In Silico Instrumental Response Correction Improves Precision of Label-free Proteomics and Accuracy of Proteomics-based Predictive Models, Lyutvinskiy et al. (2013), http://www.ncbi.nlm.nih.gov/pubmed/23589346

See Also

getRTNormFactors

Examples

```
print("No examples")
```

---

plotRTNormSummary   *Plot all retention time normalization profiles*

Description

Plot all retention time normalization profiles

Usage

```
plotRTNormSummary(eset,
  col = as.character(.getConditionColors(eset)[pData(eset)$condition, 1]),
  ...)
```

Arguments

eset	ExpressionSet
col	condition colors
...	see plot

Details

No details

Note

No note

References

In Silico Instrumental Response Correction Improves Precision of Label-free Proteomics and Accuracy of Proteomics-based Predictive Models, Lyutvinskiy et al. (2013), http://www.ncbi.nlm.nih.gov/pubmed/23589346

See Also

getRTNormFactors

Examples

```
print("No examples")
```

---

plotScoreDistrib   *Plot identifications target decoy distribution*

Description

Plot identifications target decoy distribution

Usage

```
plotScoreDistrib(targetScores, decoyScores, xlab = "Identification Score",
  ylab = "Counts", ...)
```

Arguments

targetScores	target Scores
decoyScores	decoy Scores
xlab	default "Identification Score"
ylab	default "Counts"
...	see plot

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

plotVolcano   *Plots volcano, data points colored by max cv of the 2 compared conditions*

Description

Plots volcano, data points colored by max cv of the 2 compared conditions

Usage

```
plotVolcano(obj, ratioThrs = 1, pValueThreshold = 0.01, adjusted = T, ...)
```

Arguments

`obj`	safeQuantAnalysis object or data.frame
`ratioThrs`	default 1
`pValueThreshold`	
	default 0.01
`adjusted`	TRUE/FALSE plot qValues or pValues on y-axis
`...`	see plot

Details

data.frame input object should contain 3 columns (ratio,qValue,cv)

Note

No note

References

NA

Examples

```
print("No examples")
```

`plotXYDensity`	*Scatter plot with density coloring*

Description

Scatter plot with density coloring

Usage

```
plotXYDensity(x, y, isFitLm = T, legendPos = "bottomright",
  disp = c("abline", "R", "Rc"), pch = 20, ...)
```

Arguments

`x`	number vector
`y`	number vector
`isFitLm`	fit linear model
`legendPos`	see legend
`disp`	c("abline","R","Rc") display options
`pch`	see plot
`...`	see plot

Note

No note

References

NA

Examples

```
print("No examples")
```

---

purityCorrectTMT	*Correct channel intensities based on Reporter ion Isotopic Distributions*

Description

Correct channel intensities based on Reporter ion Isotopic Distributions

Usage

```
purityCorrectTMT(tmtData, impurityMatrix = impurityMatrix)
```

Arguments

tmtData   data.frame containing tmt channel intensities

impurityMatrix correction matrix

Details

Same method as MSnbase, and described in Breitwieser et al. 2012 (Book Chapter)

Value

data.frame of corrected tmt intensities

Note

No note

References

NA

Examples

```
print("No examples")
```

| removeOutliers | *Set value to NA if it deviatves with more than 1.5 * IQR from lower/upper quantile* |

Description

Set value to NA if it deviatves with more than 1.5 * IQR from lower/upper quantile

Usage

```
removeOutliers(x, na.rm = TRUE, ...)
```

Arguments

x	vector numeric
na.rm	logical indicating whether missing values should be removed.
...	qunatile args

Details

No details

Note

No note

References

NA

See Also

NA

Examples

```
print("No examples")
```

| rollUp | *Roll up feature intensites per unique colum combination* |

Description

Roll up feature intensites per unique colum combination

Usage

```
rollUp(eset, method = "sum", featureDataColumnName = c("proteinName"))
```

Arguments

`eset`	ExpressionSet
`method`	"sum", "mean" or "top3"
`featureDataColumnName`	
	vector of column names e.g. peptide or proteinName

Details

featureDataColumnName = c("peptide","charge","ptm"), method= c("sum"), sums up intensities per peptie modification charge state

Value

ExpressionSet object

Note

No note

References

No references

Examples

```
print("No examples")
```

---

rtNormalize	*Normalization data per retention time bin*

Description

Normalization data per retention time bin

Usage

```
rtNormalize(eset, rtNormFactors)
```

Arguments

`eset`	ExpressionSet
`rtNormFactors`	obtained using getRTNormFactors

Details

Normalize for variations in elelctrospray ionization current.

Value

data.frame normalization factors per retention time bin (minute)

Note

No note

References

In Silico Instrumental Response Correction Improves Precision of Label-free Proteomics and Accuracy of Proteomics-based Predictive Models, Lyutvinskiy et al. (2013), `http://www.ncbi.nlm.nih.gov/pubmed/23589346`

See Also

`getRTNormFactors`

Examples

```
print("No examples")
```

---

safeQuantAnalysis   *safeQunat s3 class*

Description

safeQunat s3 class

Usage

```
safeQuantAnalysis(eset = eset, method = c("global", "naRep", "pairwise"),
  intensityAdjustmentObj = NA, fcThrs = 1)
```

Arguments

eset	ExpressionSet
method	c("global","naRep","rt","quantile","pairwise","all")
intensityAdjustmentObj	list
fcThrs	fold change threshold

---

setNbPeptidesPerProtein

Set nbPeptides coulmn of featureData

Description

Set nbPeptides coulmn of featureData

Usage

```
setNbPeptidesPerProtein(eset)
```

Arguments

eset   ExpressionSet

Details

NA

Value

eset

Note

No note

References

NA

Examples

```
print("No examples")
```

---

setNbSpectraPerProtein

Set nbPeptides coulmn of featureData

Description

Set nbPeptides coulmn of featureData

Usage

```
setNbSpectraPerProtein(eset)
```

Arguments

eset   ExpressionSet

Details

NA

Value

eset

Note

No note

References

NA

Examples

```
print("No examples")
```

---

sqNormalize   *Normalize*

Description

Normalize

Usage

```
sqNormalize(eset, method = "global")
```

Arguments

eset	ExpressionSet
method	c("global","rt","quantile")

Details

No details

Value

eset ExpressionSet

Note

No note

References

NA

See Also

getGlobalNormFactors, getRTNormFactors

Examples

```
print("No examples")
```

---

standardise   *Standardise data*

Description

Standardise data

Usage

```
standardise(d)
```

Arguments

d   vector or data.frame or matrix

Details

No details

Value

vector or data.frame or matrix

Note

No note

Examples

```
print("No examples")
```

---

stripACs   *strip uniprot format e.g. "sp|Q8CHJ2|AQP12_MOUSE" -> Q8CHJ2*

Description

strip uniprot format e.g. "sp|Q8CHJ2|AQP12_MOUSE" -> Q8CHJ2

Usage

```
stripACs(acs)
```

Arguments

acs   accession numbers

Details

TRUE if less than 10

Value

vector character

Note

No note

References

NA

Examples

```
print("No examples")
```

Index