Package 'SafeQuant'

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Type Package

Title A Toolbox for the Analysis of Proteomics Data

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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,
ggplot2,
magrittr,
UniProt.ws,
GO.db

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RoxygenNote 6.0.1

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")
```

cysteinFreqBarplot *Plot Cystein Frequency*

Description

Plot Cystein Frequency

Usage

```
cysteinFreqBarplot(peptides, ...)
```

Arguments

peptides	vector
...	see plot

Details

Selecting for peptides of length 7-19

Note

No note

References

NA

Examples

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

dotProduct *Return dotProduct of two vectors*

Description

Return dotProduct of two vectors

Usage

```
dotProduct(u, v, norm = F)
```

Arguments

u	vector 1
v	vector 2
norm	dp TRUE/FALSE

Value

dp

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")
```

---

getAccessionNumber *Extract accession numbers from Uniprot proteinNames*

Description

Extract accession numbers from Uniprot proteinNames

Usage

```
getAccessionNumber(proteinName)
```

Arguments

proteinName	vector of protein names

Details

sp|A0MZ66|SHOT1_HUMAN -> A0MZ66

Value

vector of uniprot accession numbers

Note

No note

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")
```

getAllDotProduct *Return dotProducts to most transition intensities of most intense runs*

Description

Return dotProducts to most transition intensities of most intense runs

Usage

```
getAllDotProduct(eset, nbRefRuns = 4)
```

Arguments

eset	ExpressionSet
nbRefRuns	(default top 4)

Value

dp

Note

No note

References

NA

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

data.frame of pvalues per condition comparison

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")
```

`getFTestPValue` *Perform statistical test (mderated F-test)*

Description

Perform statistical test (mderated F-test)

Usage

```
getFTestPValue(eset, adjust = F, log = T)
```

Arguments

`eset`	ExpressionSet
`adjust`	TRUE/FALSE adjust for multiple testing using Benjamini & Hochberg (1995) method
`log`	T/F log-transform expression values

Details

No details

Value

list of pvalues

Note

No note

References

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

See Also

`eBayes`

Examples

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

`getGeneName` *Extract Gene Name from uniprot fasta header description*

Description

Extract Gene Name from uniprot fasta header description

Usage

```
getGeneName(proteinDescription)
```

Arguments

`proteinDescription`	vector of descriptions

Details

ATP synthase subunit beta OS=Salmonella typhimurium (strain SL1344) GN=atpD -> atpD

Value

vector of gene names

Note

No note

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")
```

`getGoTermDF` *Get Go term data for a list of uniprot accession numbers*

Description

Get Go term data for a list of uniprot accession numbers

Usage

```
getGoTermDF(taxId = taxId, acs = acs)
```

Arguments

`taxId`	uniprot taxon identifier
`acs`	vector uniprot accession numbers

Details

NA

Value

data.frame "UNIPROTKB" "GO-ID" "ccIds" "mfIds" "bpIds" "ccTerms" "mfTerms" "bpTerms"

Note

No note

References

NA

See Also

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")
```

`getKinaseFreq` *Get kinase matching frequnecy of each phospho peptide subsequnece*

Description

Get kinase matching frequnecy of each phospho peptide subsequnece

Usage

```
getKinaseFreq(phosphoSeqs)
```

Arguments

`phosphoSeqs`	vector of phospho peptide sub sequneces 'PARVVRpSRREEEE'

Details

NA

Value

ExpressionSet object

Note

No note

References

NA

See Also

NA

Examples

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

`getKinases` *Get all kinases matching phospho peptide sub sequnece*

Description

Get all kinases matching phospho peptide sub sequnece

Usage

```
getKinases(phosphoSeq)
```

Arguments

`phosphoSeq`	scalar peptide sub sequnece 'PARVVRpSRREEEE'

Details

NA

Value

ExpressionSet object

Note

No note

References

NA

See Also

NA

Examples

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

getLOD *Return dilution curve limit of detection*

Description

Return dilution curve limit of detection

Usage

```
getLOD(dCurve, method = "blank")
```

Arguments

dCurve	data.frame
method	c("blank","low")

Value

lod

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")
```

`getMotifFreq` *Get motif matching frequnecy of each phospho peptide subsequnece*

Description

Get motif matching frequnecy of each phospho peptide subsequnece

Usage

```
getMotifFreq(phosphoSeqs)
```

Arguments

`phosphoSeqs`	vector of phospho peptide sub sequneces 'PARVVRpSRREEEE'

Details

NA

Value

ExpressionSet object

Note

No note

References

NA

See Also

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")
```

---

getSwaths *get swath sizes ensuring equal number of precurosrs per swath*

Description

get swath sizes ensuring equal number of precurosrs per swath

Usage

```
getSwaths(mzs, nbSwaths = 30, lowerOverlap = 2)
```

Arguments

mzs	precucrsor mz values
nbSwaths	default 30
lowerOverlap	default 2 lower bound overlap preceeding window

Details

No details

Value

data.frame "binMean","lower","upper","delta"

Note

No note

References

No ref

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")
```

ggDilutionCurve *Plot dilution curve*

Description

Plot dilution curve

Usage

```
ggDilutionCurve(dCurve, lod, title = "")
```

Arguments

dCurve	data.frame columns concentration, intensity
lod	limit of detection
title	plot title

Value

ggplot2

Note

No note

References

NA

Examples

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

---

ggVolcanoPlot *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

```
ggVolcanoPlot(data = data, title = "", pValueThrs = 0.05,
  log2RatioThrs = 0.5849625, thrsLineCol = "lightgrey", thrsLineLty = 2,
  xlab = "log2 ratio", ylab = "-log10 pValue", textSize = 20,
  xlim = range(data$ratio, na.rm = T), ylim = range(-log10(data$pValue),
  na.rm = T), abline = c("both"), topNlabels = 10)
```

Arguments

data	data.frame
title	default no title
pValueThrs	default 0.01
log2RatioThrs	default log2(0.5)
thrsLineCol	default "lightgrey"
xlab	default "log2 ratio"
ylab	default "-log10 pValue"
textSize	default 20
xlim	xlim
ylim	ylim
abline	c("none","both","ratio","pvalue")
topNlabels	default 10, label top proteins/peptides ordered by p-value
defalut	2

Details

data.frame input object should contain columns ("ratio","pValue","geneName","ac","cv", "description")

Value

ggplot2 object

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")
```

kinaseMotif *Kinase motifs*

Description

Human Protein Reference Database Serine/Threonine motifs http://www.hprd.org/serine_motifs The variables are as follows:

Usage

```
kinaseMotif
```

Format

A data frame with 175 rows and 2 variables:

motif kinase motif)

kinase kinase

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 30.

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")
```

plotAllGGVolcanoes *Plots volcano of all condition comparisons*

Description

Plots volcano of all condition comparisons

Usage

```
plotAllGGVolcanoes(sqa, isAdjusted = T, ...)
```

Arguments

sqa	SafeQuantAnalysis object
isAdjusted	(T/F) plot adjusted pvalues
see	ggVolcanoPlot

Details

data.frame input object should contain columns ("ratio","pValue","geneName","ac","cv", "description")

Value

ggplot2 object

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")
```

`plotLogo` *Plot sequence logo*

Description

Plot sequence logo

Usage

```
plotLogo(motif, bgPeptides = "ACDEFGHIKLMNPQRSTVWY", main = "",
  targetResidues = c("S", "T", "Y"), ic.scale = F, ...)
```

Arguments

`motif`	list of target residue centered motfis
`bgPeptides`	peptides used to calculate residue background frequency (default uniform)
`main`	see plot
`targetResidues`	default [STY]
`ic.scale`	logical. If TRUE, the height of each column is proportional to its information content. Otherwise, all columns have the same height.

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 getRTNormFactors
`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