Package 'SafeQuant'

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Author Erik Ahrne
Maintainer Erik Ahrne <erik.ahrne@unibas.ch></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, ggplot2, magrittr, UniProt.ws, GO.db, Hmisc
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R topics documented:
addIdQvalues 3 addScaffoldPTMFAnnotations 4 barplotMSSignal 5 COLORS 6 createExpDesign 6 createExpressionDataset 7 createPairedExpDesign 8 cvBoxplot 9 cysteinFreqBarplot 10 dotProduct 10 expDesignTagToExpDesign 11
export

getAAProteinCoordinates	2
getAccessionNumber	3
getAllCV	4
getAllDotProduct	5
getAllEBayes	5
getBaselineIntensity	
getCV	
getExpDesignProgenesisCsv	
getFTestPValue	
getGeneName	
getGlobalNormFactors	
getGoTermDF	
•	
getIdLevelQvals	
getImpuritiesMatrix	
getIntSumPerProtein	
getKinaseFreq	
getKinases	
getLOD	7
getLoocvFoldError	7
getMaxIndex	8
getMeanCenteredRange	8
getModifProteinCoordinates	9
getMotifFreq	0
getMotifX	1
getNbDetectablePeptides	2
getNbMisCleavages	
getNbPeptidesPerProtein	
getNbSpectraPerProtein	
getPeptides	
getRatios	
getRTNormFactors	
getScoreCutOff	
getSignalPerCondition	
getSwaths	
getTopX	
getUserOptions	_
ggDilutionCurve	
ggVolcanoPlot	_
globalNormalize	2
hClustHeatMap	3
isCon	4
isDecoy	4
isStrippedACs	5
kinaseMotif	6
maPlotSQ	6
missinValueBarplot	7
option_list	
pairsAnnot	
parseMaxQuantProteinGroupTxt	_
parseProgenesisFeatureCsv	
parseProgenesisPeptideMeasurementCsv	
parson rogenesist epituetyteasurementesv	1

addIdQvalues 3

addI	dQvalues	Add identific target-decoy		o Expi	ressionSe	et (calcul	lated bas	ed on
Index								7
	541p1100		 	 				,
	stripACs							
	standardise							
	sqNormalize							
	setNbSpectraPerPro							
	setNbPeptidesPerPr							
	safeQuantAnalysis							
	rtNormalize							
	rollUp							
	removeOutliers .							
	purityCorrectTMT							
	plotXYDensity .							
	plotScoreDistrib . plotVolcano							
	plotScoreDistrib	•						
	plotRTNorm							
	plotROC							
	plotQValueVsPValue							
	plotPrecMassError							
	plotPrecMassErrorl							
	plotNbValidDeFeat							
	plotNbIdentification							
	plotMSSignalDistri							
	plotLogo							
	plotIdScoreVsFDR							
	plotAllGGVolcanoe							
	plotAdjustedVsNor	•						
	plotAbsEstCalibrat							
	perFeatureNormaliz							
	parseScaffoldRawF							
	parseScaffoldPTMl	Report	 	 				5
	parseProgenesisPro	teinCsv	 	 				5

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")
```

 ${\tt addScaffoldPTMFAnnotations}$

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

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

barplotMSSignal 5

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

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

6 createExpDesign

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

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

create Expression Dataset

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

 $feature {\tt Annotations}$

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

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

ExpressionSet

```
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

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

cvBoxplot 9

cvBoxplot	C.V. boxplot
CVDOXPIOL	C. v. boxpioi

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

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

10 dotProduct

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

```
\begin{array}{c} \text{tag} & \text{tag} \\ \text{expDesignDefault} \\ & \text{data.frame} \end{array}
```

Details

tag: 1,2:3:4,5,6 condition is Control 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

```
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

```
{\it safeQuantAnalysis}
```

Examples

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

```
{\tt getAAProteinCoordinates}
```

Get amino acid coordinates on protein

Description

Get amino acid coordinates on protein

Usage

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

getAccessionNumber 13

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

14 getAllCV

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

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

getAllDotProduct 15

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))
```

16 getBaselineIntensity

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

getCV 17

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

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

```
{\tt getExpDesignProgenesisCsv}
```

Parse Experimental Design from Progenesis Csv Export

Description

Parse Experimental Design from Progenesis Csv Export

Usage

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

Arguments

```
\begin{tabular}{ll} file & path to progenesis csv file \\ expressionColIndices \\ & default .getProgenesisCsvExpressionColIndices(file) \\ \end{tabular}
```

Details

No details

Value

data.frame describing experimental design

Note

No note

References

NA

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

getFTestPValue 19

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

```
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

```
\begin{tabular}{ll} \textbf{proteinDescription} \\ \textbf{vector of descriptions} \\ \end{tabular}
```

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")
```

 ${\tt getGlobalNormFactors}$

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

 $\begin{array}{ll} \text{eset} & \text{ExpressionSet} \\ \text{method} & \text{c("sum","median)} \end{array}$

getGoTermDF 21

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

22 getIBAQEset

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 sequences 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

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

getIdLevelQvals 23

 ${\tt getIdLevelQvals}$

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")
```

 ${\tt getImpuritiesMatrix}$

Get Thermo TMT impurity matrix

Description

Get Thermo TMT impurity matrix

Usage

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

24 getIntSumPerProtein

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

getKinaseFreq 25

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

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

26 getKinases

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

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

getLOD 27

getLOD

Return dilution curve limit of detection

Description

Return dilution curve limit of detection

Usage

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

Arguments

dCurve data.frame

 $\label{eq:continuous} \text{method} \qquad \qquad c(\text{"blank","low"})$

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

٧

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 modification 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

30 getMotifFreq

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

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

getMotifX 31

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

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

32 getNbMisCleavages

```
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")
```

 ${\tt getNbMisCleavages}$

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

References

No note

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

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

34 getPeptides

```
{\tt 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)
```

getRatios 35

Arguments

```
\begin{array}{ll} {\rm proteinSeq} & {\rm protein\, sequence} \\ {\rm proteaseRegExp} & {\rm protease\, Regular\, Expression} \\ {\rm nbMiscleavages} & {\rm default\, 0} \\ \end{array}
```

Details

No details

Value

vector of peptides

Note

No note

Examples

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

 ${\tt getRatios}$

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

36 getRTNormFactors

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

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

getScoreCutOff 37

 ${\tt getScoreCutOff}$

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")
```

38 getSwaths

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

getTopX 39

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

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

40 ggDilutionCurve

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

ggVolcanoPlot 41

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
                  default no title
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")
                  default 10, label top proteins/peptides ordered by p-value
topNlabels
defalut
                  2
```

42 globalNormalize

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

```
\begin{array}{ll} \texttt{eset} & \texttt{ExpressionSet} \\ \texttt{globalNormFactors} & \texttt{globalNormFactors} \end{array}
```

Details

No details

Value

eset ExpressionSet

Note

No note

References

NA

hClustHeatMap 43

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

 ${\tt conditionColors}$

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

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

isDecoy

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

isStrippedACs 45

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. "splQ8CHJ2|AQP12_MOUSE"

Usage

isStrippedACs(acs)

Arguments

acs

accession numbers

Details

TRUE if less than 10

Value

boolean TRUE/FALSE

Note

No note

References

NA

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

46 maPlotSQ

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

missinValueBarplot 47

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

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

48 pairsAnnot

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")
```

 $\verb"parseMaxQuantProteinGroupTxt"$

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

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

 ${\tt parseProgenesisFeatureCsv}$

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

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

```
parse Progenesis Peptide Measurement Csv\\
```

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)

 ${\tt expressionColIndices}$

default .getProgenesisCsvExpressionColIndices()

uniqueProteins T/F keep unique peptides only

Details

No details

Value

ExpressionSet object

Note

No note

References

NA

See Also

ExpressionSet

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

 ${\tt parseProgenesisProteinCsv}$

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

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

```
{\tt 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
                  c("formula", "lowess", "stats")
dispElements
xlab
                  xlab
ylab
                  ylab
predictorName
                  predictorName
text
                  add names beside each dot
                  expansion factor for axis labels
cex.lab
                  expansion factor for axis
cex.axis
                  expansion factor for legend
cex.text
cex.dot
                  expansion factor for plotted dots
main
                  main
                  see plot
. . .
```

Note

No note

References

NA

Examples

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

 $\verb|plotAdjustedVsNonAdjustedRatio||$

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

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

plotAllGGVolcanoes 57

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")
```

 ${\tt plotExpDesign}$

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")
```

58 plotIdScoreVsFDR

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

plotLogo 59

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

```
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")
```

```
{\tt 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

```
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), ...)
```

plotROC

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

plotRTNorm 65

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
```

```
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
```

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

plotScoreDistrib 67

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, ...)
```

68 plotXYDensity

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 vectory number vectorisFitLm fit linear modellegendPos see legend

disp c("abline","R","Rc") display options

pch see plot ... see plot

Note

No note

purityCorrectTMT 69

References

NA

Examples

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

purityCorrectTMT

Correct channel intensities based on Reporter ion Isotopic Distribu-

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

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

70 rollUp

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 deviatives 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"))
```

rtNormalize 71

Arguments

eset ExpressionSet

method "sum", "mean" or "top3"

 $feature {\tt Data} {\tt ColumnName}$

vector of column names e.g. peptide or proteinName

Details

 $feature Data Column Name = c("peptide", "charge", "ptm"), \ method = c("sum"), \ sums \ up \ intensities per peptie modification charge state$

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

 ${\tt rtNormFactors} \quad obtained \ using \ getRTNormFactors$

Details

Normalize for variations in elelctrospray ionization current.

Value

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

72 safeQuantAnalysis

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")
```

 ${\tt safeQuantAnalysis}$

safeQunat s3 class

Description

```
safeQunat s3 class
```

Usage

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

Arguments

```
\begin{tabular}{ll} eset & ExpressionSet \\ method & c("global","naRep","rt","quantile","pairwise","all) \\ intensityAdjustmentObj \\ ... \\ \end{tabular}
```

.

fcThrs fold change threshold

```
{\tt 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

Expression Set

74 sqNormalize

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

 ${\tt method}$

c("global","rt","quantile")

Details

No details

Value

eset ExpressionSet

Note

No note

References

NA

standardise 75

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

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

76 stripACs

stripACs

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

Description

```
strip uniprot format e.g. "splQ8CHJ2lAQP12_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

*Topic datasets	getIntSumPerProtein, 24
COLORS, 6	getKinaseFreq, 25
kinaseMotif,46	getKinases, 26
option_list,48	getLOD, 27
*Topic normalization	getLoocvFoldError, 27
getGlobalNormFactors, 20	getMaxIndex, 28
getLoocvFoldError, 27	getMeanCenteredRange, 28
globalNormalize,42	getModifProteinCoordinates, 29
removeOutliers, 70	getMotifFreq, 30
sqNormalize,74	getMotifX, 31
	getNbDetectablePeptides, 32
addIdQvalues, 3	getNbMisCleavages, 32
addScaffoldPTMFAnnotations, 4	getNbPeptidesPerProtein, 33
	getNbSpectraPerProtein, 34
barplotMSSignal, 5	getPeptides, 34
	getRatios, 35
COLORS, 6	getRTNormFactors, 36, 65, 66, 72
createExpDesign, 6	getScoreCutOff, 37
createExpressionDataset, 7	getSignalPerCondition, 37
createPairedExpDesign, 8	getSwaths, 38
cvBoxplot, 9	getTopX, 39
cysteinFreqBarplot, 10	getUserOptions, 40
dat Draduct 10	ggDilutionCurve, 40
dotProduct, 10	ggVolcanoPlot, 41
eBayes, <i>16</i> , <i>19</i>	globalNormalize, 42
expDesignTagToExpDesign, 11	grobalitor marize, 12
export, 12	hClustHeatMap, 43
ExpressionSet, 7, 8, 49–52, 54	,
Expressionset, 7, 6, 49–32, 34	isCon, 44
getAAProteinCoordinates, 12	isDecoy, 44
getAccessionNumber, 13	isStrippedACs,45
getAllCV, 14	
getAllDotProduct, 15	kinaseMotif, 46
getAllEBayes, 15	
getBaselineIntensity, 16	maPlotSQ, 46
getCV, 14, 17	missinValueBarplot, 47
getExpDesignProgenesisCsv, 18	anting list 40
getFTestPValue, 19	option_list, 48
getGeneName, 20	pairsAnnot, 48
getGlobalNormFactors, 20	parseMaxQuantProteinGroupTxt, 49
getGoTermDF, 21	parseProgenesisFeatureCsv, 50
getIBAQEset, 22	parseProgenesisPeptideMeasurementCsv,
getIdAQESet, 22 getIdLevelQvals, 4, 23	51
_	
<pre>getImpuritiesMatrix, 23</pre>	parseProgenesisProteinCsv, 52

78 INDEX

```
parseScaffoldPTMReport, 53
parseScaffoldRawFile, 53
perFeatureNormalization, 54
\verb|plotAbsEstCalibrationCurve|, 55|
plotAdjustedVsNonAdjustedRatio, 56
plotAllGGVolcanoes, 57
plotExpDesign, 57
plotIdScoreVsFDR, 58
plotLogo, 59
{\tt plotMSSignalDistributions}, 60
plotNbIdentificationsVsRT, 60
plotNbValidDeFeaturesPerFDR, 61
plotPrecMassErrorDistrib, 62
plotPrecMassErrorVsScore, 63
plotQValueVsPValue, 63
plotROC, 64
plotRTNorm, 65
plotRTNormSummary, 66
plotScoreDistrib,67
plotVolcano, 67
plotXYDensity, 68
purityCorrectTMT, 69
removeOutliers, 70
rollUp, 70
rtNormalize, 71
safeQuantAnalysis, 12, 72
setNbPeptidesPerProtein, 73
{\tt setNbSpectraPerProtein}, 73
sqNormalize, 74
standardise, 75
stripACs, 76
```