

# 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

**License** GPL-3

**RoxygenNote** 5.0.1

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---

addIdQvalues	<i>Add identification leve q-values to ExpressionSet (calculated based on target-decoy score distribution)</i>
--------------	--

---

**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")
```

---

calibrationCurve	<i>S3 class object describing a calibration curve and storing some figures of merit</i>
------------------	---

---

**Description**

S3 class object describing a calibration curve and storing some figures of merit

**Usage**

```
calibrationCurve(eset, method = "blank")
```

**Arguments**

eset	ExpressionSet
method	to calculate Limit of Detection / Limit of Quantification. c("blank","low")

**Details**

No details

**Value**

calibrationCurve object

**Note**

No note

**References**

Statistical characterization of multiple-reaction monitoring mass spectrometry (MRM-MS) assays for quantitative proteomics, Mani et al. (2012), <http://www.ncbi.nlm.nih.gov/pubmed/23176545>

**Examples**

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

---

COLORS	<i>color vector</i>
--------	---------------------

---

**Description**

color vector

**Usage**

COLORS

**Format**

An object of class character of length 668.

---

createExpDesign	<i>Create Experimental Design</i>
-----------------	-----------------------------------

---

**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	<i>Create Paired Expdesign</i>
-----------------------	--------------------------------

---

**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	<i>C.V. boxplot</i>
-----------	---------------------

---

**Description**

C.V. boxplot

**Usage**

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

**Arguments**

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

**Details**

No details

**Note**

No note

**References**

NA

**Examples**

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

---

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

---

### Description

Create experimental design data.frame from user input string

### Usage

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

### Arguments

tag	tag
expDesignDefault	
	data.frame

### Details

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

### Value

data.frame describing experimental design

### Note

No note

### References

NA

### Examples

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

---

export	<i>Export content of safeQuantAnalysis object</i>
--------	---

---

**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	<i>Get amino acid coordinates on protein</i>
-------------------------	--

---

**Description**

Get amino acid coordinates on protein

**Usage**

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

**Arguments**

peptideSeq	peptide sequence
proteinSeq	protein sequence
aaRegExpr	target AA reg exp

**Details**

NA

**Value**

vector of protein coordinates (mmodification residue number)

**Note**

No note

**References**

NA

**Examples**

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

---

getAllCV	<i>Calculate Coefficient of Variance per feature (Relative standard Deviation) per Condition</i>
----------	--

---

**Description**

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

**Usage**

```
getAllCV(eset)
```

**Arguments**

eset	ExpressionSet
------	---------------

**Details**

$CV = sd / mean$

**Value**

data.frame of CVs per condition

**Note**

No note

**References**

NA

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

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

---

getAllEBayes	<i>Perform statistical test (mderated t-test), comparing all case to control</i>
--------------	--

---

**Description**

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

**Usage**

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

**Arguments**

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

**Details**

No details

**Value**

ExpressionSet object

**Note**

No note

**References**

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

**See Also**[eBayes](#)

**Examples**

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

---

getBaselineIntensity	<i>Get signal at zscore x (x standard deviations below mean)</i>
----------------------	--

---

**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	<i>Calculate Coefficient of Variance per feature (Relative standard Deviation)</i>
-------	--

---

**Description**

Calculate Coefficient of Variance per feature (Relative standard Deviation)

**Usage**

```
getCV(data)
```

**Arguments**

data	data.frame of replicate signals
------	---------------------------------

**Details**

CV = sd / mean

**Value**

vector of CVs

**Note**

No note

**References**

NA

**Examples**

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

---

`getExpDesignProgenesisCsv`*Parse Experimental Design from Progenesis Csv Export*

---

**Description**

Parse Experimental Design from Progenesis Csv Export

**Usage**

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

**Arguments**

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

**Details**

No details

**Value**

data.frame describing experimental design

**Note**

No note

**References**

NA

**Examples**

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

---

getGlobalNormFactors	<i>Get normalization factors. calculated as summed/median signal per run (column) over summed/median of first run.</i>
----------------------	--

---

**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")
```



---

getIBAQset	<i>Calculate intensity-based absolute-protein-quantification (iBAQ) metric per protein</i>
------------	--

---

**Description**

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

**Usage**

```
getIBAQset(eset, proteinDB = NA, peptideLength = c(5, 36),  
  nbMisleavages = 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)
nbMisleavages	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	<i>Calculates identification level q-values based on target-decoy score distributions</i>
-----------------	---

---

**Description**

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

**Usage**

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

**Arguments**

scores	peptide/protein identificationscore
isDecoy	vector of TRUE/FALSE

**Details**

$q\text{-value} = (\text{Nb. Decoy Entries at idScore Threshold } S^*) / (\text{Nb. Target Entries at idScore Threshold } S).$  (\* idScore >= S)

**Value**

vector of q.values

**Note**

No note

**References**

NA

**Examples**

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

---

getImpuritiesMatrix	<i>Get Thermo TMT impurity matrix</i>
---------------------	---------------------------------------

---

**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	<i>Sum up raw intensities per protein and channel. keep track of number of summed spectra and unique peptides</i>
---------------------	---

---

**Description**

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

**Usage**

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

**Arguments**

intData                      data.frame of intensities per channel  
proteinACs                    vector of protein accession numbers  
peptides                      vector of peptide sequneces  
minNbPeptPerProt              minimal number of peptides per protein

**Details**

NA

No details

**Value**

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

**Note**

No note

**References**

NA

**Examples**

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

---

getLoocvFoldError	<i>Leave-One-Out Cross Validate Qunatification Model</i>
-------------------	--

---

**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	<i>get index of max in vecotr of numeric values</i>
-------------	---

---

**Description**

get index of max in vecotr of numeric values

**Usage**

```
getMaxIndex(v)
```

**Arguments**

v	vector
---	--------

---

getMeanCenteredRange	<i>Get modification coordinates on protein</i>
----------------------	--

---

**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

## References

NA

## Examples

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

---

`getMotifX`*Create motif-x peptide annotation*

---

**Description**

Create motif-x peptide annotation

**Usage**

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

**Arguments**

<code>modifPos</code>	vector positions
<code>peptide</code>	peptide sequence
<code>proteinSeq</code>	protein sequence
<code>motifLength</code>	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**

<code>peptides</code>	list of peptides
<code>peptideLength</code>	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**

<code>peptide</code>	character vector
<code>protease</code>	regular expression



**Details**

NA

**Value**

vector of integers

**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**

<code>eset</code>	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  
nbMisleavages   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	<i>Get retentiontime base normalization factors</i>
------------------	---

---

## 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	<i>Get score cutoff for a given fdr cut-off</i>
----------------	---

---

**Description**

Get score cutoff for a given fdr cut-off

**Usage**

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

**Arguments**

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

**Details**

NA

**Value**

scoreCutoff

**Note**

No note

**References**

NA

**Examples**

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

---

getSignalPerCondition	<i>Summarize replicate signal per condition (min)</i>
-----------------------	---

---

**Description**

Summarize replicate signal per condition (min)

**Usage**

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

**Arguments**

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

**Details**

No details

**Value**

data.frame of per condition signals

**Note**

No note

**References**

NA

**Examples**

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

---

getTopX

*Calculate Mean of X most intense features*

---

**Description**

Calculate Mean of X most intense features

**Usage**

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

**Arguments**

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

**Details**

No details

**Value**

vector of topX intensities per column (sample)

**Note**

No note

## References

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

## Examples

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

---

getUserOptions	<i>Read User Specified Command Line Options</i>
----------------	---

---

## Description

Read User Specified Command Line Options

## Usage

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

## Arguments

version	Safequant version number
---------	--------------------------

## Details

No details

## Value

user options list

## Note

No note

## References

NA

## Examples

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

---

globalNormalize	<i>Normalize, Norm factors calculated as median signal per run (column) over median of first run.</i>
-----------------	---

---

**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	<i>Hierarchical clustering heat map, cluster by runs intensity, features by ratio and display log2 ratios to control median</i>
---------------	---

---

**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	<i>Check if protein is a contaminant entry</i>
-------	--

---

**Description**

Check if protein is a contaminant entry

**Usage**

```
isCon(ac)
```

**Arguments**

ac	vector of protein accession numbers
----	-------------------------------------

**Details**

contaminants proteins are typically annotated as: CON\_P0000

**Value**

vector TRUE/FALSE

**Note**

No note

**References**

NA

**Examples**

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

---

isDecoy	<i>Check if protein is a decoy entry</i>
---------	--

---

**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	<i>Check if ACs are in "non-stripped" uniprot format e.g. "sp Q8CHJ2 AQP12_MOUSE"</i>
---------------	---

---

**Description**

Check if ACs are in "non-stripped" uniprot format e.g. "sp|Q8CHJ2|AQP12\_MOUSE"

**Usage**

```
isStrippedACs(acs)
```

**Arguments**

acs	accession numbers
-----	-------------------

**Details**

TRUE if less than 10

**Value**

boolean TRUE/FALSE

**Note**

No note

**References**

NA

**Examples**

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

---

maPlotSQ	<i>ma-plot</i>
----------	----------------

---

**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	<i>Plot Percentage of Features with with missing values</i>
--------------------	---

---

**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	<i>Command Line Option List</i>
-------------	---------------------------------

---

**Description**

Command Line Option List

**Usage**

```
option_list
```

**Format**

An object of class list of length 29.

---

pairsAnnot	<i>Plot lower triangle Pearsons <math>R^2</math>. Diagonal text, upper triangle all against all scatter plots with lm abline</i>
------------	--

---

## 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**

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

**Details**

No details

**Value**

ExpressionSet object

**Note**

No note

**References**

NA

**See Also**

[ExpressionSet](#)

**Examples**

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



---

`parseProgenesisPeptideMeasurementCsv`*Parse Progenesis Peptide Measurement Csv Export*

---

**Description**

Parse Progenesis Peptide Measurement Csv Export

**Usage**

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

**Arguments**

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

**Details**

No details

**Value**

ExpressionSet object

**Note**

No note

**References**

NA

**See Also**

[ExpressionSet](#)

**Examples**

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

---

`parseProgenesisProteinCsv`*Parse Progenesis Protein Csv*

---

**Description**

Parse Progenesis Protein Csv

**Usage**

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

**Arguments**

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

**Details**

No details

**Value**

ExpressionSet object

**Note**

No note

**References**

NA

**See Also**

[ExpressionSet](#)

**Examples**

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

---

`parseScaffoldPTMReport`*Parse scaffold PTM Spectrum Report*

---

**Description**

Parse scaffold PTM Spectrum Report

**Usage**

```
parseScaffoldPTMReport(file)
```

**Arguments**

file	path to Scaffold file
------	-----------------------

**Details**

No details

**Value**

data.frame

**Note**

No note

**References**

NA

**Examples**

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

---

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

---

**Description**

Parse scaffold output .xls file (RAW export)

**Usage**

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

**Arguments**

file	path to Scaffold file
expDesign	experimental design data.frame
keepFirstAcOnly	TRUE/FALSE If multiple ACs in Accession.Numbers filed. Then keep the first one only
isPurityCorrect	do purity correction

**Details**

No details

**Value**

ExpressionSet object

**Note**

No note

**References**

NA

**See Also**

[ExpressionSet](#)

**Examples**

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

---

perFeatureNormalization

*Per Feature Normalization*

---

**Description**

Per Feature Normalization

**Usage**

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

**Arguments**

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

**Details**

Example Usage: Normalize phospho peptide signals for Protein Changes

**Value**

ExpressionSet object

**Note**

No note

**References**

No references

**Examples**

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

---

```
plotAbsEstCalibrationCurve
```

*Plot absolut Estimation calibration Curve*

---

**Description**

Plot absolut Estimation calibration Curve

**Usage**

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

**Arguments**

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

**Note**

No note

**References**

NA

**Examples**

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

---

```
plotAdjustedVsNonAdjustedRatio
```

*Plot adjusted tmt ratios vs original ratios*

---

**Description**

Plot adjusted tmt ratios vs original ratios

**Usage**

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

**Arguments**

ratio	data.frame
unAdjustedRatio	data.frame

**Details**

plot adjusted tmt ratios vs original ratios

**Note**

No note

**References**

NA

**Examples**

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

---

plotExpDesign	<i>Display experimental design, high-lighting the control condition</i>
---------------	---

---

**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	<i>Plot FDR vs. identification score</i>
------------------	--

---

**Description**

Plot FDR vs. identification score

**Usage**

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

**Arguments**

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

**Details**

No details

**Note**

No note

**References**

NA

**Examples**

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

---

plotMSSignalDistributions  
*Plot ms.signal distributions*

---

**Description**

Plot ms.signal distributions

**Usage**

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

**Arguments**

d	matrix of ms-signals
col	color
ylab	default "Frequency"
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 differentially Abundant Features (applying ratio cutoff) vs. qValue/pValue for all conditions*

---

**Description**

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

**Usage**

```
plotNbValidDeFeaturesPerFDR(sqa, upRegulated = T, log2RatioCufOff = log2(1),  
  pvalRange = c(0, 0.3), pvalCutOff = 1, isLegend = T, isAdjusted = T,  
  ylab = "Nb. Features", ...)
```

**Arguments**

<code>sqa</code>	SafeQuantAnalysis Object
<code>upRegulated</code>	TRUE/FALSE select for upregulated features
<code>log2RatioCufOff</code>	log2 ratio cut-off
<code>pvalRange</code>	pValue/qValue range
<code>pvalCutOff</code>	pValue/qValue cut-off
<code>isLegend</code>	TRUE/FALSE display legend
<code>isAdjusted</code>	TRUE/FALSE qValues/pValue on x-axis
<code>ylab</code>	default Nb. Features
<code>...</code>	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**

<code>eset</code>	ExpressionSet
<code>pMassTolWindow</code>	Precursor Mass Error Tolerance Window
<code>...</code>	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	<i>Plot qValue vs pValue</i>
--------------------	------------------------------

---

**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	<i>Plot all retention time profile overalying ratios</i>
------------	--

---

## 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	ExprssionSet
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	<i>Plot all retention time normalization profiles</i>
-------------------	---

---

## 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	<i>Plot identifications target decoy distribution</i>
------------------	---

---

**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	<i>Plots volcano, data points colored by max cv of the 2 compared conditions</i>
-------------	--

---

**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	<i>Scatter plot with density coloring</i>
---------------	---

---

**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	<i>Correct channel intensities based on Reporter ion Isotopic Distributions</i>
------------------	---

---

## 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	<i>Set value to NA if it deviates with more than 1.5 * IQR from lower/upper quantile</i>
----------------	--

---

**Description**

Set value to NA if it deviates 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.
...	quantile args

**Details**

No details

**Note**

No note

**References**

NA

**See Also**

NA

**Examples**

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

---

rollUp	<i>Roll up feature intensities per unique column combination</i>
--------	--

---

**Description**

Roll up feature intensities per unique column 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	<i>Normalization data per retention time bin</i>
-------------	--

---

**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	<i>safeQunat s3 class</i>
-------------------	---------------------------

---

**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 coulumn of featureData*

---

**Description**

Set nbPeptides coulumn of featureData

**Usage**

```
setNbPeptidesPerProtein(eset)
```

**Arguments**

eset	ExpressionSet
------	---------------

**Details**

NA

**Value**

eset

**Note**

No note

**References**

NA

**Examples**

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

---

`setNbSpectraPerProtein`*Set nbPeptides coulumn of featureData*

---

**Description**

Set nbPeptides coulumn of featureData

**Usage**

```
setNbSpectraPerProtein(eset)
```

**Arguments**

eset	ExpressionSet
------	---------------

**Details**

NA

**Value**

eset

**Note**

No note

**References**

NA

**Examples**

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

---

sqNormalize	<i>Normalize</i>
-------------	------------------

---

**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	<i>Standardise data</i>
-------------	-------------------------

---

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")
```

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