# Package 'SafeQuant'

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**Type** Package

**Title** A Toolbox for the Analysis of Proteomics Data

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

**Imports** limma,
gplots,
seqinr,
corrplot,
optparse,
data.table,
epiR,
Biobase,
ggplot2,
magrittr

**License** GPL-3

**RoxygenNote** 5.0.1

## R topics documented:

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

---

## Description

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

## Usage

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

## Arguments

| | |
|---|---|
| `eset` | ExpressionSet |

## Details

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

No details

## Value

ExpressionSet object

## Note

No note

## See Also

getIdLevelQvals

## Examples

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

---

`addScaffoldPTMFAnnotations` *Add scaffold ptm annotaitons to tmt experiment*

---

## Description

Add scaffold ptm annotaitons to tmt experiment

## Usage

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

## Arguments

| | |
|---|---|
| `eset` | ExpressionSet |
| `file` | path to Scaffold file |

## Value

ExpressionSet object

## Note

No note

## References

No references

## Examples

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

barplotMSSignal *Barplot of ms-signal per column*

## Description

Barplot of ms-signal per column

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

NA

## Examples

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

## COLORS *color vector*

### Description

color vector

### Usage

```
COLORS
```

### Format

An object of class `character` of length 668.

## createExpDesign *Create Experimental Design*

### Description

Create Experimental Design

### Usage

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

### Arguments

| | |
|---|---|
| `tag` | user input tag e.g. 1,2,3:4,5,6 indicating two condition with 3 reps each |
| `nbPlex` | tmt 6 or 10 plex |

### Details

The first listed condition is always the control condition

No details

### Value

expDesign data.frame

### Note

No note

### References

NA

### Examples

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

createExpressionDataset *Create ExpressionSet object*

## Description

Create ExpressionSet object

## Usage

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

## Arguments

| | |
|---|---|
| expressionMatrix | matrix of expression signals per feature and sample |
| expDesign | experimental design data.frame |
| featureAnnotations | data.frame including e.g: Protein Description, Id score etc. |

## Details

No details

## Value

ExpressionSet object

## Note

No note

## References

NA

## See Also

ExpressionSet

## Examples

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

createPairedExpDesign *Create Paired Expdesign*

## Description

Create Paired Expdesign

## Usage

```
createPairedExpDesign(eset)
```

## Arguments

| | |
|---|---|
| eset | ExpressionSet |

## Details

Add subject colum to phenoData design data.frame

## Value

ExpressionSet object

## Note

No note

## References

NA

## See Also

ExpressionSet

## Examples

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

cvBoxplot *C.V. boxplot*

## Description

C.V. boxplot

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

NA

## Examples

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

`dotProduct` *Return dotProduct of two vectors*

## Description

Return dotProduct of two vectors

## Usage

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

## Arguments

| | |
|---|---|
| `u` | vector 1 |
| `v` | vector 2 |
| `norm` | dp TRUE/FALSE |

## Value

dp

## Note

No note

## References

NA

## Examples

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

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

## Description

Create experimental design data.frame from user input string

## Usage

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

## Arguments

| | |
|---|---|
| `tag` | tag |
| `expDesignDefault` | data.frame |

### Details

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

### Value

data.frame describing experimental design

### Note

No note

### References

NA

### Examples

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

---

## export *Export content of safeQuantAnalysis object*

---

### Description

Export content of safeQuantAnalysis object

### Usage

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

### Arguments

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

### Details

NA

### Note

No note

### References

NA

### See Also

safeQuantAnalysis

## Examples

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

---

`getAAProteinCoordinates` *Get amino acid coordinates on protein*

---

## Description

Get amino acid coordinates on protein

## Usage

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

## Arguments

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

## Details

NA

## Value

vector of protein coordinates (mmodification residue number)

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

```
getAllCV(eset)
```

## Arguments

| | |
|---|---|
| `eset` | ExpressionSet |

## Details

CV = sd / mean

## Value

data.frame of CVs per condition

## Note

No note

## References

NA

## See Also

`getCV`

## Examples

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

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

### Description

Return dotProducts to most transition intensities of most intense runs

### Usage

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

### Arguments

| | |
|---|---|
| eset | ExpressionSet |
| nbRefRuns | (default top 4) |

### Value

dp

### Note

No note

### References

NA

### Examples

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

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

### Description

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

### Usage

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

### Arguments

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

### Details

No details

### Value

ExpressionSet object

### Note

No note

### References

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

### See Also

eBayes

### Examples

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

---

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

---

### Description

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

### Usage

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

### Arguments

| | |
|---|---|
| intensities | refrence run signals |
| promille | baseline value set as specified promille |

### Value

baseline value

## Note

No note

## References

NA

## Examples

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

---

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

---

## Description

Calculate Coefficiant of Variance per feature (Relative standard Deviation)

## Usage

```
getCV(data)
```

## Arguments

| | |
|---|---|
| `data` | data.frame of replicate signals |

## Details

CV = sd / mean

## Value

vector of CVs

## Note

No note

## References

NA

## Examples

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

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

## Description

Parse Experimental Design from Progenesis Csv Export

## Usage

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

## Arguments

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

## Details

No details

## Value

data.frame describing experimental design

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

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

## Arguments

| | |
|---|---|
| `eset` | ExpressionSet |
| `method` | c("sum","median) |

## Details

No details

## Value

vector of normalization factors

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

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

### Arguments

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

### Details

No details

### Value

ExpressionSet

### Note

No note

### References

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

### Examples

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

---

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

---

### Description

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

### Usage

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

### Arguments

| | |
|---|---|
| scores | peptide/protein identficationscore |
| isDecoy | vector of TRUE/FALSE |

## Details

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

## Value

vector of q.values

## Note

No note

## References

NA

## Examples

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

---

`getImpuritiesMatrix` *Get Thermo TMT impurity matrix*

---

## Description

Get Thermo TMT impurity matrix

## Usage

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

## Arguments

| | |
|---|---|
| `plexNb` | integer, 6 or 10 plex |

## Details

No details

## Value

impurity matrix matrix

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

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

## Arguments

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

## Details

NA

No details

## Value

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

## Note

No note

## References

NA

## Examples

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

## getLOD *Return dilution curve limit of detection*

### Description

Return dilution curve limit of detection

### Usage

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

### Arguments

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

### Value

lod

### Note

No note

### References

NA

### Examples

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

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

### Description

Leave-One-Out Cross Validate Qunatification Model

### Usage

```
getLoocvFoldError(df)
```

### Arguments

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

### Details

No details

## Value

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

## Note

No note

## References

NA

## See Also

NA

## Examples

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

---

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

---

## Description

get index of max in vecotr of numeric values

## Usage

```
getMaxIndex(v)
```

## Arguments

| | |
|---|---|
| v | vector |

---

`getMeanCenteredRange` *Get modification coordinates on protein*

---

## Description

Get modification coordinates on protein

## Usage

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

## Arguments

| | |
|---|---|
| d | numeric vector |
| nbSd | range spanning number of sd frmo mean |

## Details

NA

## Value

vector range boundries

## Note

No note

## References

NA

## Examples

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

---

`getModifProteinCoordinates` *Get modification coordinates on protein*

---

## Description

Get modification coordinates on protein

## Usage

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

## Arguments

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

## Details

NA

## Value

vector of protein coordinates (mmodification residue number)

## Note

No note

## References

NA

## Examples

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

---

`getMotifX` *Create motif-x peptide annotation*

---

## Description

Create motif-x peptide annotation

## Usage

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

## Arguments

| | |
|---|---|
| `modifPos` | vector positions |
| `peptide` | peptide sequence |
| `proteinSeq` | protein sequence |
| `motifLength` | motif flanking sequence |

## Details

motif-x example PGDYS*TTPG

## Value

vector of motifs

## Note

No note

## References

NA

## Examples

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

## getNbDetectablePeptides *Get number peptides passing defined length criteria*

### Description

Get number peptides passing defined length criteria

### Usage

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

### Arguments

| | |
|---|---|
| peptides | list of peptides |
| peptideLength | vector of two integers defining peptide length range |

### Details

No details

### Value

integer corresponding to number of detectable peptides

### Note

No note

### Examples

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

## getNbMisCleavages *Get number of mis-cleavages perp peptide*

### Description

Get number of mis-cleavages perp peptide

### Usage

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

### Arguments

| | |
|---|---|
| peptide | character vector |
| protease | regular expression |

## Details

NA

## Value

vector ofintegers

## Note

No note

## References

NA

## Examples

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

---

`getNbPeptidesPerProtein` *Get number of peptides per protein*

---

## Description

Get number of peptides per protein

## Usage

```
getNbPeptidesPerProtein(eset)
```

## Arguments

| | |
|---|---|
| `eset` | ExpressionSet |

## Details

NA

## Value

table

## Note

No note

## References

NA

## Examples

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

## getNbSpectraPerProtein *Get number of spectra per protein*

### Description

Get number of spectra per protein

### Usage

```
getNbSpectraPerProtein(eset)
```

### Arguments

| | |
|---|---|
| eset | ExpressionSet |

### Details

NA

### Value

table

### Note

No note

### References

NA

### Examples

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

## getPeptides *Digest protein*

### Description

Digest protein

### Usage

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

### Arguments

| | |
|---|---|
| proteinSeq | protein sequence |
| proteaseRegExp | protease Regular Expression |
| nbMiscleavages | default 0 |

### Details

No details

### Value

vector of peptides

### Note

No note

### Examples

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

---

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

---

### Description

Calculate ratios, comparing all case to control

### Usage

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

### Arguments

| | |
|---|---|
| eset | ExpressionSet |
| method | median, mean, paired |
| log2 | transform |

### Details

No details

### Value

ExpressionSet object

### Note

No note

## References

NA

## Examples

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

---

`getRTNormFactors` *Get retentiontime base normalization factors*

---

## Description

Get retentiontime base normalization factors

## Usage

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

## Arguments

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

## Details

No details

## Value

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

## Note

No note

## References

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

## Examples

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

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

### Description

Get score cutoff for a given fdr cut-off

### Usage

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

### Arguments

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

### Details

NA

### Value

scoreCutoff

### Note

No note

### References

NA

### Examples

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

## getSignalPerCondition *Summarize replicate signal per condition (min)*

### Description

Summarize replicate signal per condition (min)

### Usage

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

### Arguments

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

### Details

No details

### Value

data.frame of per condition signals

### Note

No note

### References

NA

### Examples

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

---

## getTopX *Calculate Mean of X most intense features*

---

### Description

Calculate Mean of X most intense features

### Usage

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

### Arguments

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

### Details

No details

### Value

vector of topX intensities per column (sample)

### Note

No note

## References

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

## Examples

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

---

# getUserOptions *Read User Specified Command Line Options*

---

## Description

Read User Specified Command Line Options

## Usage

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

## Arguments

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

## Details

No details

## Value

user options list

## Note

No note

## References

NA

## Examples

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

`ggDilutionCurve` *Plot dilution curve*

## Description

Plot dilution curve

## Usage

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

## Arguments

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

## Value

ggplot

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

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

## Arguments

| | |
|---|---|
| `eset` | ExpressionSet |
| `globalNormFactors` | globalNormFactors |

### Details

No details

### Value

eset ExpressionSet

### Note

No note

### References

NA

### See Also

getGlobalNormFactors

### Examples

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

---

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

---

### Description

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

### Usage

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

### Arguments

| | |
|---|---|
| eset | ExpressionSet |
| conditionColors | data.frame of colors per condition |
| breaks | default seq(-2,2,length=20) |
| dendogram | see heatmap.2 gplots |
| legendPos | see legend |
| ... | see plot |

### Details

No details

## Note

No note

## References

NA

## Examples

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

---

`isCon` *Check if protein is a contaminant entry*

---

## Description

Check if protein is a contaminant entry

## Usage

```
isCon(ac)
```

## Arguments

| | |
|---|---|
| `ac` | vector of protein accession numbers |

## Details

contanminants proteins are typically annotated as: CON_P0000

## Value

vector TRUE/FALSE

## Note

No note

## References

NA

## Examples

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

## isDecoy *Check if protein is a decoy entry*

### Description

Check if protein is a decoy entry

### Usage

```
isDecoy(ac)
```

### Arguments

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

### Details

decoy proteins are typically annotated as: REV_P0000

### Value

vector TRUE/FALSE

### Note

No note

### References

NA

### Examples

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

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

### Description

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

### Usage

```
isStrippedACs(acs)
```

### Arguments

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

### Details

TRUE if less than 10

### Value

boolean TRUE/FALSE

### Note

No note

### References

NA

### Examples

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

---

## maPlotSQ *ma-plot*

---

### Description

ma-plot

### Usage

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

### Arguments

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

### Note

No note

### References

NA

## Examples

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

---

`missinValueBarplot` *Plot Percentage of Features with with missing values*

---

## Description

Plot Percentage of Features with with missing values

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

NA

## Examples

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

## option_list *Command Line Option List*

### Description

Command Line Option List

### Usage

```
option_list
```

### Format

An object of class `list` of length 29.

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

### Description

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

### Usage

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

### Arguments

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

### Details

No details

### Note

No note

## References

NA

## Examples

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

---

`parseMaxQuantProteinGroupTxt` *Parse MaxQuant Protein Group Txt*

---

## Description

Parse MaxQuant Protein Group Txt

## Usage

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

## Arguments

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

## Details

No details

## Value

ExpressionSet object

## Note

No note

## References

NA

## See Also

`ExpressionSet`

## Examples

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

parseProgenesisFeatureCsv *Parse Progenesis Feature Csv Export*

## Description

Parse Progenesis Feature Csv Export

## Usage

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

## Arguments

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

## Details

No details

## Value

ExpressionSet object

## Note

No note

## References

NA

## See Also

ExpressionSet

## Examples

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

`parseProgenesisPeptideMeasurementCsv` *Parse Progenesis Peptide Measurement Csv Export*

## Description

Parse Progenesis Peptide Measurement Csv Export

## Usage

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

## Arguments

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

## Details

No details

## Value

ExpressionSet object

## Note

No note

## References

NA

## See Also

`ExpressionSet`

## Examples

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

`parseProgenesisProteinCsv` *Parse Progenesis Protein Csv*

## Description

Parse Progenesis Protein Csv

## Usage

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

## Arguments

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

## Details

No details

## Value

ExpressionSet object

## Note

No note

## References

NA

## See Also

`ExpressionSet`

## Examples

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

parseScaffoldPTMReport *Parse scaffold PTM Spectrum Report*

## Description

Parse scaffold PTM Spectrum Report

## Usage

```
parseScaffoldPTMReport(file)
```

## Arguments

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

## Details

No details

## Value

data.frame

## Note

No note

## References

NA

## Examples

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

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

## Description

Parse scaffold output .xls file (RAW export)

## Usage

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

### Arguments

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

### Details

No details

### Value

ExpressionSet object

### Note

No note

### References

NA

### See Also

ExpressionSet

### Examples

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

---

## perFeatureNormalization

*Per Feature Normalization*

---

### Description

Per Feature Normalization

### Usage

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

### Arguments

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

## Details

Example Usage: Normalize phospho peptide signals for Protein Changes

## Value

ExpressionSet object

## Note

No note

## References

No references

## Examples

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

---

`plotAbsEstCalibrationCurve`
*Plot absolut Estimation calibration Curve*

---

## Description

Plot absolut Estimation calibration Curve

## Usage

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

## Arguments

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

## Note

No note

## References

NA

## Examples

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

---

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

---

## Description

Plot adjusted tmt ratios vs original ratios

## Usage

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

## Arguments

| | |
|---|---|
| `ratio` | data.frame |
| `unAdjustedRatio` | data.frame |

## Details

plot adjusted tmt ratios vs original ratios

## Note

No note

## References

NA

## Examples

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

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

### Description

Display experimental design, high-lighting the control condition

### Usage

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

### Arguments

| | |
|---|---|
| eset | ExpressionSet |
| condColors | condition colors |
| version | version number |

### Details

No details

### Note

No note

### References

NA

### Examples

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

## plotIdScoreVsFDR *Plot FDR vs. identification score*

### Description

Plot FDR vs. identification score

### Usage

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

### Arguments

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

### Details

No details

### Note

No note

### References

NA

### Examples

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

---

## plotMSSignalDistributions

*Plot ms.signal distributions*

---

### Description

Plot ms.signal distributions

### Usage

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

### Arguments

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

### Details

No details

## Note

No note

## References

NA

## Examples

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

---

`plotNbIdentificationsVsRT` *Plot the number of identified Features per Reteintion Time minute.*

---

## Description

Plot the number of identified Features per Reteintion Time minute.

## Usage

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

## Arguments

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

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

NA

## Examples

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

`plotPrecMassErrorDistrib` *Plot Precursor Mass Error Distribution*

## Description

Plot Precursor Mass Error Distribution

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

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

### Arguments

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

### Details

No details

### Note

No note

### References

NA

### Examples

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

---

## plotQValueVsPValue *Plot qValue vs pValue*

---

### Description

Plot qValue vs pValue

### Usage

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

### Arguments

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

### Details

No details

### Note

No note

### References

NA

### Examples

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

plotROC *Plot Number of Identifications vs. FDR*

## Description

Plot Number of Identifications vs. FDR

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

NA

## Examples

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

`plotRTNorm` *Plot all retention time profile overalying ratios*

## Description

Plot all retention time profile overalying ratios

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

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

## See Also

`getRTNormFactors`

## Examples

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

`plotRTNormSummary` *Plot all retention time normalization profiles*

## Description

Plot all retention time normalization profiles

## Usage

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

## Arguments

| | |
|---|---|
| `eset` | ExpressionSet |
| `col` | condition colors |
| `...` | see plot |

## Details

No details

## Note

No note

## References

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

## See Also

`getRTNormFactors`

## Examples

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

## plotScoreDistrib *Plot identifications target decoy distribution*

### Description

Plot identifications target decoy distribution

### Usage

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

### Arguments

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

### Details

No details

### Note

No note

### References

NA

### Examples

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

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

### Description

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

### Usage

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

### Arguments

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

### Details

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

### Note

No note

### References

NA

### Examples

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

---

## plotXYDensity *Scatter plot with density coloring*

---

### Description

Scatter plot with density coloring

### Usage

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

### Arguments

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

### Note

No note

## References

NA

## Examples

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

---

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

---

## Description

Correct channel intensities based on Reporter ion Isotopic Distributions

## Usage

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

## Arguments

| | |
|---|---|
| `tmtData` | data.frame containing tmt channel intensities |
| `impurityMatrix` | correction matrix |

## Details

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

## Value

data.frame of corrected tmt intensities

## Note

No note

## References

NA

## Examples

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

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

## Description

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

## Usage

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

## Arguments

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

## Details

No details

## Note

No note

## References

NA

## See Also

NA

## Examples

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

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

## Description

Roll up feature intensites per unique colum combination

## Usage

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

### Arguments

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

### Details

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

### Value

ExpressionSet object

### Note

No note

### References

No references

### Examples

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

---

## rtNormalize *Normalization data per retention time bin*

---

### Description

Normalization data per retention time bin

### Usage

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

### Arguments

| | |
|---|---|
| eset | ExpressionSet |
| rtNormFactors | obtained using getRTNormFactors |

### Details

Normalize for variations in elelctrospray ionization current.

### Value

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

## Note

No note

## References

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

## See Also

getRTNormFactors

## Examples

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

---

# safeQuantAnalysis *safeQunat s3 class*

---

## Description

safeQunat s3 class

## Usage

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

## Arguments

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

setNbPeptidesPerProtein *Set nbPeptides coulmn of featureData*

## Description

Set nbPeptides coulmn of featureData

## Usage

```
setNbPeptidesPerProtein(eset)
```

## Arguments

| | |
|---|---|
| eset | ExpressionSet |

## Details

NA

## Value

eset

## Note

No note

## References

NA

## Examples

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

setNbSpectraPerProtein *Set nbPeptides coulmn of featureData*

## Description

Set nbPeptides coulmn of featureData

## Usage

```
setNbSpectraPerProtein(eset)
```

## Arguments

| | |
|---|---|
| eset | ExpressionSet |

### Details

NA

### Value

eset

### Note

No note

### References

NA

### Examples

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

---

`sqNormalize` *Normalize*

---

### Description

Normalize

### Usage

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

### Arguments

| | |
|---|---|
| `eset` | ExpressionSet |
| `method` | c("global","rt","quantile") |

### Details

No details

### Value

eset ExpressionSet

### Note

No note

### References

NA

## See Also

getGlobalNormFactors, getRTNormFactors

## Examples

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

---

`standardise` *Standardise data*

---

## Description

Standardise data

## Usage

```
standardise(d)
```

## Arguments

| | |
|---|---|
| `d` | vector or data.frame or matrix |

## Details

No details

## Value

vector or data.frame or matrix

## Note

No note

## Examples

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

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

## Description

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

## Usage

```
stripACs(acs)
```

## Arguments

| | |
|---|---|
| `acs` | accession numbers |

## Details

TRUE if less than 10

## Value

vector character

## Note

No note

## References

NA

## Examples

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

# Index