

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,
epiR,
Biobase,
ggplot2,
ggrepel,
magrittr,
Hmisc,
pcaMethods,
impute,
dplyr,
GO.db,
UniProt.ws,
data.table,
affy

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R topics documented:

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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")
```

| | |
|--------|---------------------|
| 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

| | |
|---------------------------------|--|
| <code>expressionMatrix</code> | matrix of expression signals per feature and sample |
| <code>expDesign</code> | experimental design data.frame |
| <code>featureAnnotations</code> | 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 | <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")
```

| | |
|--------------------|-------------------------------|
| cysteinFreqBarplot | <i>Plot Cystein Frequency</i> |
|--------------------|-------------------------------|

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 | <i>Return dotProduct of two vectors</i> |
|------------|---|

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 | <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")
```

| | |
|--------------------|--|
| getAccessionNumber | <i>Extract accession numbers from Uniprot proteinNames</i> |
|--------------------|--|

Description

Extract accession numbers from Uniprot proteinNames

Usage

```
getAccessionNumber(proteinName)
```

Arguments

| | |
|-------------|-------------------------|
| proteinName | vector of protein names |
|-------------|-------------------------|

Details

splA0MZ66|SHOT1_HUMAN -> A0MZ66

Value

vector of uniprot accession numbers

Note

No note

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")
```

| | |
|------------------|---|
| getAlldotProduct | <i>Return dotProducts to most transition intensities of most intense runs</i> |
|------------------|---|

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")
```

| | |
|--------------|--|
| getAlIEBayes | <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

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

Arguments

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

Details

No details

Value

data.frame of pvalues per condition comparison

Note

No note

References

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

See Also

[eBayes](#)

Examples

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

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

Description

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

Usage

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

Arguments

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

Value

baseline value

Note

No note

References

NA

Examples

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

| | |
|-------|--|
| getCV | <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")
```

| | |
|----------------|---|
| getFTestPValue | <i>Perform statistical test (mderated F-test)</i> |
|----------------|---|

Description

Perform statistical test (mderated F-test)

Usage

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

Arguments

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

Details

No details

Value

list of pvalues

Note

No note

References

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

See Also

[eBayes](#)

Examples

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

| | |
|-------------|--|
| getGeneName | <i>Extract Gene Name from uniprot fasta header description</i> |
|-------------|--|

Description

Extract Gene Name from uniprot fasta header description

Usage

```
getGeneName(proteinDescription)
```

Arguments

```
proteinDescription
      vector of descriptions
```

Details

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

Value

vector of gene names

Note

No note

Examples

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

| | |
|----------------------|--|
| getGlobalNormFactors | <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")
```

`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

| | |
|--------------------|----------------------------------|
| <code>taxId</code> | uniprot taxon identifier |
| <code>acs</code> | vector uniprot accession numbers |

Details

NA

Value

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

Note

No note

References

NA

See Also

NA

Examples

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

| | |
|------------|--|
| 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),
  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, Schwanhauser (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")
```

getImputationMatrix *Get matrix of imputed valeus in ExpressionSet matrix*

Description

Get matrix of imputed valeus in ExpressionSet matrix

Usage

```
getImputationMatrix(eset, method = "intensity")
```

Arguments

eset ExpressionSet
method c("intensity","count") default intensity

Value

matrix

Note

No note

See Also

No note

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 sequences |
| minNbPeptPerProt | minimal number of peptides per protein |

Details

NA
No details

Value

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

Note

No note

References

NA

Examples

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

| | |
|---------------|--|
| getKinaseFreq | <i>Get kinase matching frequency of each phospho peptide subsequence</i> |
|---------------|--|

Description

Get kinase matching frequency of each phospho peptide subsequence

Usage

```
getKinaseFreq(phosphoSeqs)
```

Arguments

phosphoSeqs vector of phospho peptide sub sequences 'PARVVRpSRREEEE'

Details

NA

Value

ExpressionSet object

Note

No note

References

NA

See Also

NA

Examples

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

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

Description

Get all kinases matching phospho peptide sub sequence

Usage

```
getKinases(phosphoSeq)
```

Arguments

`phosphoSeq` scalar peptide sub sequence 'PARVVRpSRREEEE'

Details

NA

Value

ExpressionSet object

Note

No note

References

NA

See Also

NA

Examples

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

| | |
|--------|---|
| getLOD | <i>Return dilution curve limit of detection</i> |
|--------|---|

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 | <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 vecotor of numeric values</i> |
|-------------|--|

Description

get index of max in vecotor 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 boundaries

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

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

Details

NA

Value

vector of protein coordinates (mmodification residue number)

Note

No note

References

NA

Examples

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

| | |
|--------------|---|
| getMotifFreq | <i>Get motif matching frequency of each phospho peptide subsequence</i> |
|--------------|---|

Description

Get motif matching frequency of each phospho peptide subsequence

Usage

```
getMotifFreq(phosphoSeqs)
```

Arguments

phosphoSeqs vector of phospho peptide subsequences 'PARVVVRpSRREEEEE'

Details

NA

Value

ExpressionSet object

Note

No note

References

NA

See Also

NA

Examples

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

| | |
|-----------|-----------------------------------|
| getMotifX | Create motif-x peptide annotation |
|-----------|-----------------------------------|

Description

Create motif-x peptide annotation

Usage

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

Arguments

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

Details

motif-x example PGDYS*TTPG

Value

vector of motifs

Note

No note

References

NA

Examples

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

| | |
|---------------|--|
| getNAFraction | <i>Get fraction missing values per ratio/condition/run</i> |
|---------------|--|

Description

Get fraction missing values per ratio/condition/run

Usage

```
getNAFraction(eset, method = c("ratio", "intensity"))
```

Arguments

| | |
|--------|---|
| eset | ExpressionSet |
| method | c("ratio","cond","run","count","intensity") |

Value

matrix

Note

No note

See Also

No note

Examples

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

| | |
|-------------------------|--|
| getNbDetectablePeptides | <i>Get number peptides passing defined length criteria</i> |
|-------------------------|--|

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 | <i>Get number of mis-cleavages perp peptide</i> |
|-------------------|---|

Description

Get number of mis-cleavages perp peptide

Usage

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

Arguments

| | |
|----------|--------------------|
| peptide | character vector |
| protease | 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

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

Details

NA

Value

table

Note

No note

References

NA

Examples

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

`getNbRolledUpFeatures` *Get number rolled up features per row*

Description

Get number rolled up features per row

Usage

```
getNbRolledUpFeatures(eset, method = "vector")
```

Arguments

| | |
|--------|-------------------------------------|
| eset | ExpressionSet |
| method | c("vector","matrix") default vector |

Value

matrix

Note

No note

See Also

No note

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 | <i>Digest protein</i> |
|-------------|-----------------------|

Description

Digest protein

Usage

```
getPeptides(proteinSeq, proteaseRegExp = .getProteaseRegExp("trypsin"),  
            nbMisleavages = 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 | <i>Calculate ratios, comparing all case to control</i> |
|-----------|--|

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 | <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 *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, sum |

Details

No details

Value

data.frame of per condition signals

Note

No note

References

NA

Examples

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

| | |
|-----------|---|
| getSwaths | <i>get swath sizes ensuring equal number of precurosr per swath</i> |
|-----------|---|

Description

get swath sizes ensuring equal number of precurosr per swath

Usage

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


Arguments

| | |
|--------------|---|
| mzs | precursor mz values |
| nbSwaths | default 30 |
| lowerOverlap | default 2 lower bound overlap preceeding window |

Details

No details

Value

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

Note

No note

References

No ref

Examples

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

getTopX

Calculate Mean of X most intense features

Description

Calculate Mean of X most intense features

Usage

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

Arguments

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

Details

No details

Value

vector of topX intensities per column (sample)

Note

No note

References

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

Examples

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

| | |
|----------------|---|
| getUserOptions | <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")
```

| | |
|-----------------|----------------------------|
| ggDilutionCurve | <i>Plot dilution curve</i> |
|-----------------|----------------------------|

Description

Plot dilution curve

Usage

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

Arguments

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

Value

ggplot2

Note

No note

References

NA

Examples

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

| | |
|---------------|--|
| ggVolcanoPlot | <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

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

Arguments

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

Details

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

Value

ggplot2 object

Note

No note

References

NA

Examples

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

| | |
|-----------------|---|
| globalNormalize | <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

contaminant 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")
```

| | |
|-------------|----------------------|
| kinaseMotif | <i>Kinase motifs</i> |
|-------------|----------------------|

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

| | |
|-----------------------|--------------------|
| <code>eset</code> | ExpressionSet |
| <code>sample</code> | selected condition |
| <code>cex.lab</code> | default 1.5 |
| <code>cex.axis</code> | default 1.5 |
| <code>lwd</code> | default 2 |
| <code>pch</code> | default 1 |
| <code>col</code> | green transparent |
| <code>...</code> | 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

| | |
|-----------------------|---------------|
| <code>eset</code> | ExpressionSet |
| <code>col</code> | col |
| <code>cex.axis</code> | cex.axis |
| <code>cex.lab</code> | cex.lab |
| <code>...</code> | see plot |

Details

No details

Note

No note

References

NA

Examples

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

| | |
|--------------------------|---------------------------------|
| <code>option_list</code> | <i>Command Line Option List</i> |
|--------------------------|---------------------------------|

Description

Command Line Option List

Usage

```
option_list
```

Format

An object of class `list` of length 31.

| | |
|------------|--|
| pairsAnnot | <i>Plot lower triangle Pearsons R^2. 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), exclusivePeptides = F)
```

Arguments

| | |
|-----------------------------------|---|
| <code>file</code> | path to Progenesis Peptide Measurement csv file |
| <code>expDesign</code> | experimental design data.frame |
| <code>method</code> | auc (area under curve) or spc (spectral count) |
| <code>expressionColIndices</code> | default .getProgenesisCsvExpressionColIndices() |
| <code>specificPeptides</code> | T/F keep specific 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

| | |
|------------------------------|-------------------------|
| <code>ratio</code> | <code>data.frame</code> |
| <code>unAdjustedRatio</code> | <code>data.frame</code> |

Details

plot adjusted tmt ratios vs original ratios

Note

No note

References

NA

Examples

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

| | |
|--------------------|---|
| plotAllGGVolcanoes | <i>Plots volcano of all condition comparisons</i> |
|--------------------|---|

Description

Plots volcano of all condition comparisons

Usage

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

Arguments

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

Details

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

Value

ggplot2 object

Note

No note

References

NA

Examples

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

| | |
|---------------|---|
| plotExpDesign | <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")
```

| | |
|----------|---------------------------|
| plotLogo | <i>Plot sequence logo</i> |
|----------|---------------------------|

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

Note

No note

References

NA

Examples

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

```
plotMSSignalDistributions
  Plot ms.signal distributions
```

Description

Plot ms.signal distributions

Usage

```
plotMSSignalDistributions(d, col = 1:100, ylab = "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),
  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 | 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")
```

 rollUpDT

Roll up feature intensites per unique colum combination

Description

Roll up feature intensites per unique colum combination

Usage

```
rollUpDT(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 electrospray 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 | <i>Set nbPeptides coulmn of featureData</i> |
|-------------------------|---|

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 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")
```

`sqImpute`*Impute missing values*

Description

Impute missing values

Usage

```
sqImpute(eset, method = "gmin", rowmax = 0.3)
```

Arguments

| | |
|---------------------|---|
| <code>eset</code> | ExpressionSet |
| <code>method</code> | <code>c("knn", "ppca", "gMin", lMin)</code> |
| <code>rowmax</code> | The maximum percent missing data allowed in any row to apply ppca and knn (if more missing values impute gmin). default 0.3 |

Details

- `gMin`: half global minimum (0.1 percentile)
- `lMin`: half local minimum
- `gMean`: half global mean
- `lMean`: half local mean
- `knn`: Nearest neighbour averaging, as implemented in the `impute::impute.knn` function
- `ppca`: An iterative method using a probabilistic model to handle missing values, as implemented in the `pcaMethods::pca` function.

Value

ExpressionSet

Note

No note

References

Accounting for the Multiple Natures of Missing Values in Label-Free Quantitative Proteomics Data Sets to Compare Imputation Strategies, Lazar et al (2016), <http://pubs.acs.org/doi/abs/10.1021/acs.jproteome.5b00981>

See Also

No note

Examples

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

`sqNormalize`*Normalize*

Description

Normalize

Usage

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

Arguments

| | |
|---------------------|--|
| <code>eset</code> | ExpressionSet |
| <code>method</code> | <code>c("global","rt","quantile")</code> |

Details

No details

Value

eset ExpressionSet

Note

No note

References

NA

See Also

`getGlobalNormFactors`, `getRTNormFactors`

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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