

Package ‘isobar’

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Title Analysis and quantitation of isobarically tagged MSMS proteomics data

Description isobar provides methods for preprocessing, normalization, and report generation for the analysis of quantitative mass spectrometry proteomics data labeled with isobaric tags, such as iTRAQ and TMT.

Version 1.8.1

Author Florian P Breitwieser <fbreitwieser@cemm.oeaw.ac.at> and Jacques Colinge <jcolinge@cemm.oeaw.ac.at>, with contributions from Xavier Robin <xavier.robin@unige.ch> and Florent Gluck <florent.gluck@unige.ch>

Maintainer Florian P Breitwieser <fbreitwieser@cemm.oeaw.ac.at>

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Imports distr

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URL <http://bioinformatics.cemm.oeaw.ac.at>

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isobar-package	<i>Analysis and quantitation of isobarically tagged MSMS proteomics data</i>
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Description

isobar provides methods for preprocessing, normalization, and report generation for the analysis of quantitative mass spectrometry proteomics data labeled with OA isobaric tags, such as iTRAQ and TMT.

Details

Package: isobar
 Version: 1.1.2
 biocViews: Proteomics, MassSpectrometry, Bioinformatics, MultipleComparisons, QualityControl
 Depends: R (>= 2.9.0), Biobase, stats, methods, ggplot2
 Imports: distr, biomaRt
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 URL: <http://bioinformatics.cemm.oeaw.ac.at>
 Collate: utils.R ProteinGroup-class.R IBSpectra-class.R NoiseModel-class.R ratio-methods.R sharedpep-methods.R MS

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Further information is available in the following vignettes:

isobar	Isobar Overview (source, pdf)
isobar-devel	Isobar for developers (source, pdf)

Author(s)

Florian P Breitwieser <fbreitwieser@cemm.oeaw.ac.at> and Jacques Colinge <jcolinge@cemm.oeaw.ac.at>, with contributions from Xavier Robin <xavier.robin@unige.ch>

Maintainer: Florian P Breitwieser <fbreitwieser@cemm.oeaw.ac.at>

calc.delta.score *Calculate Delta Score from Ion Score*

Description

Calculates delta score from raw search engine score by subtracting the best matching hit with the second best matching. data needs to have not only the best hit per spectrum, but multiple, to be able to calculate the delta score. filterSpectraDeltaScore calls calc.delta.score and filters spectra below a minum delta score.

Usage

```
calc.delta.score(my.data)
filterSpectraDeltaScore(my.data, min.delta.score=10, do.remove=FALSE)
```

Arguments

my.data	IBSpectra data frame.
min.delta.score	Minimum delta score.
do.remove	If TRUE, spectra below the min.prob threshold are not just set as 'use.for.quant=FALSE' but removed.

Value

Returns data with additional column 'delta.score'.

Author(s)

Florian P. Breitwieser

calcPeptidePosition *Recalculate peptide start positions based on protein sequence*

Description

Function to recalculate start position of peptide in protein when it is missing or wrong.

Usage

```
calcPeptidePosition(peptide.info, protein.info, calc.il.peptide)
```

Arguments

peptide.info	Peptide info object of ProteinGroup.
protein.info	Protein info object of ProteinGroup.
calc.il.peptide	Should the 'real' peptide (I/L difference) be calculated?

calculate-pvalues *Calculate and Adjust Ratio and Sample p-values.*

Description

Functions for calculating and adjusting ratios and sample p-values. Usually, these are called by proteinRatios or peptideRatios.

Usage

```
calculate.ratio.pvalue(lratio, variance, ratiodistr = NULL)
calculate.sample.pvalue(lratio, ratiodistr)

calculate.mult.sample.pvalue(lratio, ratiodistr, strict.pval,
                             lower.tail, n.possible.val, n.observed.val)

adjust.ratio.pvalue(quant.tbl, p.adjust, sign.level.rat, globally = FALSE)
```

Arguments

lratio	log 10 protein or peptide ratios.
ratiodistr	Fitted ratio distribution/
variance	Variance of lratios.
strict.pval	If FALSE, missing ratios are ignored. If TRUE, missing ratios are penalized by giving them a sample.pval of 0.5.
lower.tail	lower.tail of distribution?

n.possible.val Number of possible ratios.
 n.observed.val Number of observed ratios.
 quant.tbl Quantification table (from proteinRatios or peptideRatios).
 p.adjust p-value adjustment method (see ?p.adjust).
 sign.level.rat Ratio significance level.
 globally Whether the p-values should be adjusted over all conditions, or individually in each condition.

Author(s)

Florian P. Breitwieser

See Also

[proteinRatios](#), [peptideRatios](#)

Examples

```
lratio <- c(-1,-1,seq(from=-1,to=1,by=.25),1,1)
variance <- c(0,1,rep(0.1,9),0,1)
ratiodistr.precise <- new("Norm",mean=0,sd=.25)
ratiodistr.wide <- new("Norm",mean=0,sd=.5)

# ratio p-value is impacted only by the variance
# sample p-value captures whether the ratio distribution is narrow (precise)
# or wide
data.frame(lratio, variance,
           ratio.pvalue=calculate.ratio.pvalue(lratio, variance),
           sample.pvalue.precise=calculate.sample.pvalue(lratio,ratiodistr.precise),
           sample.pvalue.wide=calculate.sample.pvalue(lratio,ratiodistr.wide))
```

calculate.dNSAF *dNSAF approximate abundance calculations.*

Description

Distributed normalized spectral abundance factor (dNSAF) is a label free quantitative measure of protein abundance based on spectral counts which are corrected for peptides shared by multiple proteins. Original publication: Zhang Y et al., Analytical Chemistry (2010).

Usage

```
calculate.dNSAF(protein.group, use.mw = FALSE, normalize = TRUE,
               combine.f = mean)
```

Arguments

protein.group	ProteinGroup object. Its @proteinInfo slot data.frame must contain a length column.
use.mw	Use MW to account for protein size
normalize	Normalize dSAF to dNSAF?
combine.f	How to handle proteins seen only with shared peptides?

Value

Named numeric vector of dNSAF values.

Author(s)

Florian P Breitwieser

References

Zhang Y et al., Analytical Chemistry (2010)

See Also

[proteinInfo](#), [getProteinInfoFromUniprot](#), [calculate.emPAI](#), [ProteinGroup](#)

Examples

```
data(ibspiked_set1)
protein.group <- proteinGroup(ibspiked_set1)
calculate.dNSAF(protein.group)
```

calculate.emPAI	<i>emPAI approximate abundance calculations.</i>
-----------------	--

Description

The Exponentially Modified Protein Abundance Index (emPAI) is a label free quantitative measure of protein abundance based on protein coverage by peptide matches. The original publication is Ishihama Y, et al., Proteomics (2005).

Usage

```
calculate.emPAI(protein.group, protein.g = reporterProteins(protein.group), normalize = FALSE,
  observed.pep = c("pep", "mod.charge.pep"), use.mw = FALSE, combine.f = mean,
  ..., nmc = 0, report.all = FALSE)
n.observable.peptides(...)
observable.peptides(seq, nmc = 1, min.length = 6, min.mass = 600, max.mass = 4000,
  custom = list(code = c("B", "Z", "J", "U"),
    mass = c(164.554862, 278.61037, 213.12392, 150.953636)), ...)
```

Arguments

protein.group	ProteinGroup object. Its @proteinInfo slot data.frame must contain a sequence column to calculate the number of observable peptides per protein.
protein.g	Protein group identifiers.
normalize	Normalize to sum = 1?.
observed.pep	What counts as observed peptide?
report.all	TOADD
use.mw	Use MW to normalize for protein size
combine.f	How to handle proteins seen only with shared peptides?
seq	Protein sequence.
nmc	Number of missed cleavages.
min.length	Minimum length of peptide.
min.mass	Minimum mass of peptide.
max.mass	Maximum mass of peptide.
custom	User defined residue for Digest .
...	Further arguments to observable.peptides/Digest .

Details

The formula is

$$emPAI = 10^{\frac{N_{<-observed}}{N_{<-observable}}} - 1$$

$N_{<-observed}$ is the number of observed peptides - we use the count of unique peptide without consideration of charge state. $N_{<-observable}$ is the number of observable peptides. Sequence cleavage is done using [Digest](#).

Value

Named numeric vector of emPAI values.

Author(s)

Florian P Breitwieser

References

Ishihama Y, et al., Proteomics (2005)

See Also

[Digest](#), [proteinInfo](#), [getProteinInfoFromUniprot](#), [calculate.dNSAF](#), [ProteinGroup](#)

Examples

```
data(ibspiked_set1)
protein.group <- proteinGroup(ibspiked_set1)
calculate.emPAI(protein.group,protein.g=protein.g(protein.group,"CERU"))
```

 correct.peptide.ratios

Correct peptide ratios with protein ratios from a separate experiment.

Description

Correct peptide ratios with protein ratios from a separate experiment.

Usage

```
correct.peptide.ratios(ibspectra, peptide.quant.tbl, protein.quant.tbl, adjust.variance = TRUE, corre
```

Arguments

ibspectra	IBSpectra object.
peptide.quant.tbl	Calculated with peptideRatios.
protein.quant.tbl	Calculated with proteinRatios.
adjust.variance	Adjust variance of ratios.
correlation	Assumed correlation between peptide and protein ratios for variance adjustment.
recalculate.pvalue	Recalculate p-value after variance adjustment.

Author(s)

Florian P. Breitwieser

 distr-methods

Functions for distribution calculations

Description

calcProbXGreaterThanY calculates the probability that $P(X) > P(Y) + .5 P(X)=P(Y)$. calcProbXDiffNormals calculates the probabilities of a set of normals, defined by the vectors mu_Y and sd_Y are greater or less than the reference distribution Y.

Usage

```
calcProbXGreaterThanY(X, Y, min.q = 10^-6, n.steps = 1000)
calcProbXDiffNormals(X, mu_Y, sd_Y, ..., alternative = "greater")
distrprint(X, round.digits = 5)
twodistr.plot(X, Y, n.steps = 1000, min.q = 10^-3)
```

Arguments

X	Object of the class Distribution.
Y	Object of the class Distribution.
min.q	minimum quantile
n.steps	Number of steps.
mu_Y	Numeric vector of parameter mu of a Normal.
sd_Y	Numeric vector of parameter sd of a Normal.
...	Additional arguments to calcProbXGreaterThanY.
alternative	"less", "greater", or "two-sided".
round.digits	Round digits for printing.

Author(s)

Florian P. Breitwieser

Examples

```
calcProbXGreaterThanY(Norm(0, .25), Norm(1, .25))
```

fit distributions *Fit weighted and unweighted Cauchy and Normal distributions*

Description

Functions to fit the probability density functions on ratio distribution.

Usage

```
fitCauchy(x)
fitNorm(x, portion = 0.75)
fitWeightedNorm(x, weights)
fitNormalCauchyMixture(x)
fitGaussianMixture(x, n = 500)
fitGumbel(x)
fitTltd(x)
```

Arguments

x	Ratios
weights	Weights
portion	Central portion of data to take for computation
n	number of sampling steps

Value

Cauchy, Norm

Author(s)

Florian P Breitwieser, Jacques Colinge.

See Also

[proteinRatios](#)

Examples

```
library(distr)
data(ibspiked_set1)
data(noise.model.hcd)
# calculate protein ratios of Trypsin and CERU_HUMAN. Note: this is only
# for illustration purposes. For estimation of sample variability, data
# from all protein should be used
pr <- proteinRatios(ibspiked_set1, noise.model=noise.model.hcd,
                    cl=as.character(c(1,1,2,2)), combn.method="intraClass", protein=c("136429", "P00450"))

# fit a Cauchy distribution
ratiodistr <- fitCauchy(pr$lratio)
plot(ratiodistr)
```

getPeptideModifContext

Get context of modification

Description

Gets neighboring amino acids around modification which can be used to find enriched motifs.

Usage

```
getPeptideModifContext(protein.group, modif, n.aa.up = 5, n.aa.down = 5)
```

Arguments

protein.group	ProteinGroup object.
modif	Modification of interest.
n.aa.up	Number of AA downstream to report.
n.aa.down	Number of AA upstream to report.

```
getPhosphoRSProbabilities
```

Generate input files for PhosphoRS, call it, and get modification site probabilities

Description

Get phosphorylation site localization probabilities by calling PhosphoRS and parsing its output. `getPhosphoRSProbabilities` generates a XML input file for PhosphoRS calling `writePhosphoRSInput`, then executes `phosphoRS.jar` with `java`, and parses the XML result file with `readPhosphoRSOutput`.

Usage

```
getPhosphoRSProbabilities(id.file, mgf.file, massTolerance, activationType,
                          simplify = FALSE, mapping.file = NULL, mapping =
                          c(peaklist = "even", id = "odd"), pepmodif.sep =
                          "##.##", besthit.only = TRUE, phosphors.cmd =
                          paste("java -jar", system.file("phosphors",
                          "phosphoRS.jar", package = "isobar")), file.basename =
                          tempfile("phosphors."))
```

```
writePhosphoRSInput(phosphoRS.infile, id.file, mgf.file, massTolerance,
                    activationType, mapping.file = NULL, mapping =
                    c(peaklist = "even", id = "odd"), pepmodif.sep =
                    "##.##", modif.masses = rbind(c("PHOS", "1",
                    "1:Phospho:Phospho:79.966331:PhosphoLoss:97.976896:STY"),
                    c("Oxidation_M", "2",
                    "2:Oxidation:Oxidation:15.994919:null:0:M"),
                    c("Cys_CAM", "3",
                    "3:Carbamidomethylation:Carbamidomethylation:57.021464:null:0:C"),
                    c("iTRAQ4plex", "4",
                    "4:iTRAQ4:iTRAQ4:144.1544:null:0:KX"), c("iTRAQ8plex",
                    "5", "5:iTRAQ8:iTRAQ8:304.308:null:0:KX"),
                    c("TMT6plex", "7",
                    "7:TMT6:TMT6:229.162932:null:0:KX"), c("TMTsixplex",
                    "6", "6:TMT6:TMT6:229.162932:null:0:KX")))
```

```
readPhosphoRSOutput(phosphoRS.outfile, simplify = FALSE, pepmodif.sep = "##.##", besthit.only = TRUE)
```

```
filterSpectraPhosphoRS(id.file, mgf.file, ..., min.prob = NULL, do.remove=FALSE)
```

Arguments

`id.file` Database search results file in `ibspectra.csv` or `mzIdentML` format. See [IBSpectra](#) and [isobar vignette](#) for information on converting Mascot dat and Phenyx pidres

	files into ibspectra format.
mgf.file	Peaklist file
massTolerance	Fragment ion mass tolerance (in Da)
activationType	Activation types of spectra. CID, HCD, or ETD.
simplify	If TRUE, returns a data.frame instead of a list.
mapping.file	Mapping file. See also readIBSpectra .
mapping	Mapping columns.
besthit.only	Only show best hit, simplifies result to data.frame instead of list.
phosphors.cmd	PhosphoRS script.
file.basename	Base name for creating phosphoRS input and output files.
phosphoRS.infile	PhosphoRS input XML file name.
phosphoRS.outfile	PhosphoRS output XML file name.
pepmodif.sep	separator of peptide and modification in XML id
modif.masses	masses and ID used for PhosphoRS
min.prob	Threshold for PhosphoRS peptide probability to consider it for quantification
...	Further arguments to getPhosphoRSProbabilities
do.remove	If TRUE, spectra below the min.prob threshold are not just set as 'use.for.quant=FALSE' but removed.

Details

PhosphoRS is described in Taus et al., 2011. It can be downloaded from <http://cores.imp.ac.at/protein-chemistry/download/> and used as Freeware. Java is required at runtime.

Value

If simplify=TRUE, a data.frame with the following columns: spectrum, peptide, modif, PepScore, PepProb, seqpos

If simplify=FALSE, a list (of spectra) of lists (of peptide identifications) of lists (with information about identification and localization). spectrum -> peptide 1, peptides 2, ... -> peptide. First level: - spectrum Second level: - peptide identifications for spectrum (might be more than one) Third level: - peptide: vector with peptide sequence and modification string - site.probs: matrix with site probabilities for each phospho site - isoforms: peptide score and probabilities for each isoform

Author(s)

Florian P Breitwieser

References

Taus et al., 2011

getPtmInfo

Get PTM site information for identified proteins from public databases.

Description

Get PTM site information for identified proteins from public databases.

Usage

```
getPtmInfoFromPhosphoSitePlus(protein.group, file.name = NULL, modif = "PHOS",
                               psp.url = "http://www.phosphosite.org/downloads/",
                               mapping = c(PHOS = "Phosphorylation_site_dataset.gz",
                                           ACET = "Acetylation_site_dataset.gz",
                                           METH = "Methylation_site_dataset.gz",
                                           SUMO = "Sumoylation_site_dataset.gz",
                                           UBI = "Ubiquitination_site_dataset.gz"))
```

```
getPtmInfoFromNextprot(protein.group, nextprot.url = "http://www.nextprot.org/rest/entry/NX_XXX/ptm",
                       url.wildcard = "XXX")
```

Arguments

protein.group	ProteinGroup object.
file.name	File name to save downloaded data, defaults to the original file name (see mapping).
modif	Selects dataset to download (see mapping).
psp.url	PhosphoSitePlus main URL for datasets.
mapping	Names of PhosphoSitePlus modification datasets, mapped by modif name.
nextprot.url	URL for fetching Nextprot results. url.wildcard will be replaced by the Uniprot Protein AC.
url.wildcard	wildcard to replace with Uniprot protein AC in nextprot.url.

Details

PhosphoSitePlus datasets are downloaded and written to the working directory with its original name (see mapping) unless a file with that name exists, which is then parsed into a data.frame of suitable format.

Value

data.frame with (at least) the columns: isoform_ac, description, evidence, position

Note

PhosphoSitePlus is licensed under Creative Commons Attribution-NonCommercial-ShareAlike 3.0 Unported License and is freely available for non-commercial purpose, see <http://www.phosphosite.org/staticDownloads.do>.
 neXtProt is licensed under the Creative Commons Attribution-NoDerivs License, see: <http://creativecommons.org/licenses/by-nd/3.0>.
 Please read the conditions and use the data only if you agree.

Author(s)

Florian P. Breitwieser

References

PhosphoSitePlus: a comprehensive resource for investigating the structure and function of experimentally determined post-translational modifications in man and mouse. Hornbeck PV, Kornhauser JM, Tkachev S, Zhang B, Skrzypek E, Murray B, Latham V, Sullivan M. *Nucleic Acids Res.* 2012 Jan;40(Database issue):D261-70. Epub 2011 Dec 1.

neXtProt: a knowledge platform for human proteins. Lane L, Argoud-Puy G, Britan A, Cusin I, Duek PD, Evalet O, Gateau A, Gaudet P, Gleizes A, Masselot A, Zwahlen C, Bairoch A. *Nucleic Acids Res.* 2012 Jan;40(Database issue):D76-83. Epub 2011 Dec 1.

Examples

```
## Not run:
data(ib_phospho)
ptm.info.np <- getPtmInfoFromNextprot(proteinGroup(ib_phospho))
ptm.info.np <- ptm.info.np[grep("Phospho",ptm.info.np$modification.name),]
ptm.info.psp <- getPtmInfoFromPhosphoSitePlus(proteinGroup(ib_phospho),modif="PHOS")

str(ptm.info.np)
str(ptm.info.psp)

## End(Not run)
```

groupMemberPeptides *Peptide info for protein group members*

Description

For a given reporter protein group identifier, information on its peptides is returned. It contains information on how the peptides are shared and in which member they occur.

Usage

```
groupMemberPeptides(x, reporter.protein.g, ordered.by.pos = TRUE, only.first.pos = TRUE)
```

Arguments

x ProteinGroup object
reporter.protein.g group reporter protein
ordered.by.pos if TRUE, start position of peptides in proteins is exported and peptides are ordered by position
only.first.pos if TRUE, only first occurrence of peptide in protein is reported

Value

list of two: [1] peptide.info: data.frame peptide specificity n.shared.groups n.shared.proteins start.pos
 [2] group.member.peptides: data.frame each column corresponds to a group member, and each row to a peptide

Author(s)

Florian P Breitwieser

Examples

```

data(ibspiked_set1)
protein.group <- proteinGroup(ibspiked_set1)
ceru.rat <- protein.g(protein.group, "CERU_RAT")
groupMemberPeptides(protein.group, ceru.rat)

## find protein groups with members
t <- table(proteinGroupTable(protein.group)$reporter.protein)
t[t>2]
protein.g <- names(t)[t>2][1]
groupMemberPeptides(protein.group, protein.g)
  
```

human.protein.names *Info on proteins*

Description

Gather human readable information from protein group codes.

Usage

```
my.protein.info(x, protein.g)
```

```
human.protein.names(my.protein.info)
```


Arguments

x	ProteinGroup object
protein.g	protein
my.protein.info	Return value of function my.protein.info

Author(s)

Florian P Breitwieser

IBSpectra-class	<i>IBSpectra Class for Isobarically Tagged Quantitative MS Proteomics Data</i>
-----------------	--

Description

This class represents a quantitative MS proteomics experiment labeled using Isobaric tags (iTRAQ, TMT). IBSpectra is an abstract class which is implemented in the [IBSpectraTypes](#) classes `iTRAQ4plexSpectra`, `iTRAQ8plexSpectra`, `TMT2plexSpectra`, `TMT6plexSpectra` and `TMT10plexSpectra`.

It contains per-spectrum measurements of the reporter tag intensity and m/z in `assayData`, and protein grouping in `proteinGroup`.

Objects from the Class

IBSpectra objects are typically created using the [readIBSpectra](#) method or by calls of the form `new("iTRAQ4plexSpectra", data=NULL, data.ions=NULL, ...)`.

Slots

IBSpectra extends [eSet](#) which is a container for high-throughput assays and experimental meta-data. Slots introduced in `eSet` (for more details on slots and methods refer to [eSet](#) help):

assayData: Contains matrices 'ions' and 'mass' storing reporter tag intensities and m/z values for each tag and spectrum. Can be accessed by [reporterIntensities](#) and [reporterMasses](#).
Class: [AssayData](#)

phenoData: Contains experimenter-supplied variables describing phenotypes behind reporter tags.
Class: [AnnotatedDataFrame-class](#)

featureData: Describes the spectra's retention time, charge, peptide sequence, etc and can be accessed by [fData](#). Class: [AnnotatedDataFrame](#)

experimentData: Contains details of experimental methods. Class: [MIAME](#)

annotation: UNUSED. Label associated with the annotation package used in the experiment.
Class: character

protocolData: UNUSED. Contains equipment-generated variables describing reporter tags. Class: [AnnotatedDataFrame](#)

log: character matrix logging isotope impurity correction, normalization, etc.

Slots introduced in IBSpectra:

proteinGroup: A [ProteinGroup](#) object describing peptide and protein identifications grouped by shared peptides.

reporterTagNames: A character vector denoting the reporter tag labels.

reporterMasses: The 'true' m/z of the reporter tags in the MS/MS spectrum, used to isolate m/z-intensity pairs from peaklist.

isotopeImpurities: Manufacturer supplied isotope impurities, need to be set per batch and used for correction by [correctIsotopeImpurities](#).

Constructor

See [readIBSpectra](#) for creation based on peaklist (e.g. MGF format) and identification files (Mascot and Phenyx output).

new(type, data): Creates a IBSpectra object.

type Denotes the type of IBSpectra, either 'iTRAQ4plexSpectra', 'iTRAQ8plexSpectra', 'TMT2plexSpectra', 'TMT6plexSpectra' or 'TMT10plexSpectra'. Call [IBSpectraTypes\(\)](#) to see a list of the implemented types.

data A 'data.frame' in a ibspectra-csv format.

Coercion

In the code snippets below, x is a IBSpectra object. IBSpectra object can be coerced to

as(x, "data.frame"): Creates a data.frame containing all identification and quantitation information. Peptide matching to multiple proteins produce multiple lines.

ibSpectra.as.concise.data.frame(x): Creates a data.frame containing all identification and quantitation information. Proteins are concatenated - so the resulting data.frame has one line per spectrum.

as(x, "MSnSet"): Coerces to a [MSnSet](#) object (package [MSnbase](#)).

as(msnset, "IBSpectra"): Coerces a [MSnSet](#) to IBSpectra object.

Accessors

In the following code snippets, x is a IBSpectra object.

proteinGroup(x): Gets and sets the ProteinGroup.

isotopeImpurities(x): Gets and sets the isotope impurities of the isobaric tags as defined by the manufacturers per batch.

reporterData(x, element="ions", na.rm=FALSE, na.rm.f='any', ...): Gets and sets the element ('ions' or 'mass') for each tag and spectrum. '...' is handed down to spectrumSel, so it is possible to select for peptides or proteins. If na.rm is TRUE, than spectra missing quantitative information in 'any' or 'all' channels (parameter na.rm.f) are removed.

reporterIntensities(x, ...): Convenience function, calls [reporterData\(...,element="ions"\)](#)

reporterMasses(x, ...): Convenience function, calls [reporterData\(...,element="mass"\)](#)

spectrumTitles(x, ...): Gets the spectrum titles. '...' is passed down to spectrumSel.

classLabels(x): Gets and sets the class labels in phenoData. Used for summarization, see also [estimateRatio](#) and [phenoData](#).

Methods

In the following code snippets, `x` is a `IBSpectra` object.

`subsetIBSpectra(x, protein=NULL, peptide=NULL, direction="exclude", specificity):`

Get a 'subset' of `IBSpectra`: include or exclude proteins or peptides. When selection is based on proteins, it can be defined to exclude only peptides which are specific to the protein ('reporter-specific'), specific to the group ('group-specific') or which are shared with other proteins ('unspecific'). See [subsetIBSpectra](#).

`spectrumSel(x, peptide, protein, specificity="reporter-specific"):` Gets a boolean vector selecting the corresponding spectra: If peptide is given, all spectra assigned to this peptide. If protein is given, all spectra assigned to peptides of this protein with specificity 'specificity'. See also [ProteinGroup](#).

Author(s)

Florian P. Breitwieser

See Also

[ProteinGroup](#), [isobar-preprocessing](#), [isobar-analysis](#), [isobar-plots](#)

Examples

```
data(ibspiked_set1)
ibspiked_set1
head(reporterIntensities(ibspiked_set1))
head(reporterMasses(ibspiked_set1))
proteinGroup(ibspiked_set1)
isotopeImpurities(ibspiked_set1)

# create new object
set.seed(123)
data <- data.frame(spectrum=letters,
                  peptide=sample(c("pepA", "pepB", "pepC"), 26, TRUE),
                  start.pos=1,
                  modif=sample(c("::X::", "::Y::", "::Z::"), 26, TRUE),
                  accession=c("protein1", "protein2"))
data.ions <- matrix(rnorm(26*2, 1000, 50),
                  ncol=2, dimnames=list(letters, NULL))
data.mass <- matrix(rep(c(126.1, 127.1), 26),
                  ncol=2, byrow=TRUE, dimnames=list(letters, NULL))
ib <- new("TMT2plexSpectra", data, data.ions, data.mass)
ib
reporterIntensities(ib)
isotopeImpurities(ib) <- matrix(c(0.8, 0.1, 0.2, 0.9), nrow=2)
reporterIntensities(correctIsotopeImpurities(ib))
```

`IBSpectra.log`*Log functions for IBSpectra objects*

Description

The slot `log` of `IBSpectra` objects contains a matrix with two columns which contain a timestamp and message. Rownames relate to the item logged.

Used by [correctIsotopeImpurities](#) and [normalize](#).

Usage

```
do.log(x, name, msg)
```

```
get.log(x, name)
```

```
is.logged(x, name)
```

Arguments

<code>x</code>	<code>IBSpectra</code> object
<code>name</code>	Name of property to be logged (translates to row name).
<code>msg</code>	Message to be logged for name.

Details

A warning message will be displayed if a already logged property is logged again.

Value

`do.log`: `IBSpectra` object with updated `log`. `get.log`:

Author(s)

Florian P Breitwieser

See Also

`IBSpectra-class`

Examples

```
data(ibspiked_set1)
ib <- normalize(correctIsotopeImpurities(ibspiked_set1))
ib@log
```

 Isobar util functions *Isobar util functions*

Description

Utility functions. `paste0` as a shorthand to `paste(...,sep="")` in versions of R pre 2.14.

Usage

```
paste0(..., sep = "")
a %inrange% b
```

Arguments

<code>...</code>	Arguments to paste.
<code>sep</code>	Separator.
<code>a</code>	values.
<code>b</code>	range.

Author(s)

Florian P Breitwieser

Examples

```
1:10
```

 isobar-analysis *IBSpectra analysis: Protein and peptide ratio calculation*

Description

Calculates the relative abundance of a peptide or protein in one tag compared to another.

Usage

```
estimateRatio(ibspectra, noise.model = NULL, channel1, channel2, protein, peptide, ...)
estimateRatioForPeptide(peptide, ibspectra, noise.model, channel1, channel2, combine = TRUE, ...)
estimateRatioForProtein(protein, ibspectra, noise.model, channel1, channel2, combine = TRUE, method = '

## S4 method for signature numeric,numeric,missing
estimateRatioNumeric(channel1,channel2,summarize.f=median, ...)

## S4 method for signature numeric,numeric,NoiseModel
estimateRatioNumeric(channel1,channel2,noise.model,ratiodistr=NULL,variance.function="maxi",
```

```

sign.level=0.05,sign.level.rat=sign.level,sign.level.sample
remove.outliers=TRUE,outliers.args=list(method = "iqr", outl
method="isobar",fc.threshold=1.3,
channel1.raw=NULL,channel2.raw=NULL,use.na=FALSE,preweights

## S4 method for signature IBSpectra,ANY,character,character,character,missing
estimateRatio(ibspectra,noise.model,channel1,channel2,
               protein,peptide,...)

## S4 method for signature IBSpectra,ANY,character,character,character,NULL
estimateRatio(ibspectra,noise.model,channel1,channel2,
               protein,peptide=NULL,...)

## S4 method for signature IBSpectra,ANY,character,character,missing,character
estimateRatio(ibspectra,noise.model,channel1,channel2,protein,peptide,...)
## S4 method for signature IBSpectra,ANY,character,character,NULL,character
estimateRatio(ibspectra,noise.model,channel1,channel2,protein=NULL,peptide,...)

```

Arguments

<code>ibspectra</code>	IBSpectra object.
<code>noise.model</code>	NoiseModel object.
<code>channel1</code>	Tag channel 1. Can either be a character denoting a 'reporter name' or a numeric vector whose value should be summarized. Ratio is calculated as channel2/channel1.
<code>channel2</code>	Tag channel 2. Can either be a character denoting a 'reporter name' or a numeric vector whose value should be summarized. Ratio is calculated as channel2/channel1.
<code>protein</code>	Protein(s) of interest. If present, channel1 and channel2 must be reporter names. Provide either proteins or peptides.
<code>peptide</code>	Peptide(s) of interest. If present, channel1 and channel2 must be reporter names. Provide either proteins or peptides.
<code>combine</code>	If true, a single ratio is returned even for multiple peptides/spectra. If false, a data.frame with a row for each peptide/protein is returned.
<code>specificity</code>	See specificities .
<code>quant.w.groupeptides</code>	Proteins which should be quantified with group specific peptides. Normally, only reporter specific peptides are used.
<code>ratiodistr</code>	distr object of ratio distribution.
<code>variance.function</code>	Defines how the variance for ratio is calculated. 'ev' is the estimator variance and thus 1/sum(1/variances). 'wsv' is the weighted sample variance. 'maxi' method takes the maximum of the former two variances.
<code>sign.level</code>	Significance level.

<code>sign.level.rat</code>	Signal p-value significance level.
<code>sign.level.sample</code>	Sample p-value significance level.
<code>remove.outliers</code>	Should outliers be removed?
<code>outliers.args</code>	Arguments for outlier removal, see <code>OUTLIERS</code> function (TODO).
<code>method</code>	method taken for ratio computation and selection: one of <code>'isobar'</code> , <code>'libra'</code> , <code>'multiq'</code> , <code>'pep'</code> , <code>'ttest'</code> and <code>'compare.all'</code> .
<code>fc.threshold</code>	When method equals <code>fc</code> , takes this as fold change threshold.
<code>summarize.f</code>	A method for summarizing spectrum ratios when no other information is available. For example <code>median</code> or <code>mean</code> .
<code>channel1.raw</code>	When given, noise estimation is based on <code>channel1.raw</code> and <code>channel2.raw</code> . These are the intensities of the channels before normalization.
<code>channel2.raw</code>	See <code>channel1.raw</code> .
<code>use.na</code>	Use NA values to calculate ratio. Experimental feature - use with caution.
<code>preweights</code>	Specifies weights for each spectrum. Experimental feature - use with caution.
<code>...</code>	Passed down to <code>estimateRatioNumeric</code> methods.

Value

In general, a named character vector with the following elements: - `lratio`: log ratio - variance - `n.spectra`: number of spectra available in the ratio calculation - `p.value.rat`: Signal p-value. NA if called w/o `ratiodistr` - `p.value.sample`: Sample p-value. NA if called w/o `ratiodistr` - `is.significant`: NA if called w/o `ratiodistr`

If `combine=FALSE`, `estimateRatio` returns a `data.frame`, with columns as described above.

Author(s)

Florian P. Breitwieser, Jacques Colinge

See Also

[ProteinGroup](#), [IBSpectra](#), [isobar-preprocessing](#), [isobar-plots](#) [proteinRatios](#)

Examples

```
data(ibspiked_set1)
data(noise.model.hcd)
ceru.human <- protein.g(proteinGroup(ibspiked_set1), "CERU_HUMAN")
ceru.rat <- protein.g(proteinGroup(ibspiked_set1), "CERU_RAT")
ceru.mouse <- protein.g(proteinGroup(ibspiked_set1), "CERU_MOUSE")
ceru.proteins <- c(ceru.human,ceru.rat,ceru.mouse)

## Calculate ratio based on all spectra of peptides specific
## to CERU_HUMAN, CERU_RAT or CERU_MOUSE. Returns a named
## numeric vector.
```

```

10^estimateRatio(ibspiked_set1,noise.model.hcd,
                 channel1="114",channel2="115",
                 protein=ceru.proteins)[lratio]

## If argument combine=FALSE, estimateRatio returns a data.frame
## with one row per protein
10^estimateRatio(ibspiked_set1,noise.model.hcd,
                 channel1="114",channel2="115",
                 protein=ceru.proteins,combine=FALSE)[,lratio]
## spiked material channel 115 vs 114:
##          CERU_HUMAN (P00450): 1
##          CERU_RAT   (P13635): 2
##          CERU_MOUSE (Q61147): 0.5

```

isobar-import

Loading data into IBSpectra objects using readIBSpectra

Description

Read ibspectra-csv files and peaklist files as an IBSpectra object of type 'type' (see [IBSpectra](#), e.g. iTRAQ4plexSpectra or TMT6plexSpectra). If peaklist.file is missing, it is assumed that id.file contains intensity and m/z columns for the reporter tags.

Usage

```

## S4 method for signature character,character
readIBSpectra(type,id.file)

# reads id file
## S4 method for signature character,character,character
readIBSpectra(
  type, id.file, peaklist.file, sep = "\t", mapping.file
  = NULL, mapping = c(quantification.spectrum = "hcd",
  identification.spectrum = "cid"), id.file.domap =
  NULL, identifications.format = NULL, decode.titles =
  FALSE, ...)

# reads peaklist file
## S4 method for signature character,data.frame,character
readIBSpectra(
  type, id.file, peaklist.file, annotate.spectra.f =
  NULL, peaklist.format = NULL, scan.lines = 0,
  fragment.precision = NULL, fragment.outlier.prob =
  NULL, ...)

```


Arguments

<code>type</code>	Name of class of new <code>IBSpectra</code> object: <code>iTRAQ4plexSpectra</code> , <code>iTRAQ8plexSpectra</code> , <code>TMT2plexSpectra</code> , <code>TMT6plexSpectra</code> , or <code>TMT10plexSpectra</code>
<code>id.file</code>	Database search results file in <code>ibspectra.csv</code> or <code>mzIdentML</code> format. See <code>identifications.format</code> . See the vignette for information on converting Mascot dat and Phenyx pidres files into <code>ibspectra</code> format.
<code>peaklist.file</code>	Peaklist file, typically in MGF format, see <code>peaklist.format</code> . MGF must be centroid!
<code>mapping.file</code>	If defined, spectrum titles from the peaklist file are linked to the identifications via this file. This can be used when running HCD runs for quantification and CID runs for identification. See Koecher et al., 2009 for details.
<code>mapping</code>	Named character vector defining the names of columns in <code>mapping.file</code> . The names must be 'peaklist' and 'id', and the values must correspond to colnames of the mapping files.
<code>id.file.domap</code>	When using HCD-CID or a method akin and every spectrum is used for identification, the ID result files of the HCD run can be specified in <code>id.file.domap</code> . Then, the results are merged after mapping the identification results.
<code>annotate.spectra.f</code>	Function which changes or annotates the spectra feature data before it is written to <code>IBspectra</code> object. This can be used to calculate and threshold additional scores, for example localization scores of post-translational modifications such as Delta Score (<code>filterSpectraDeltaScore</code>) or PhosphoRS site localization probabilities (<code>annotateSpectraPhosphoRS</code>).
<code>peaklist.format</code>	"mgf" (Mascot Generic format) or "mcn" (iTracker Machine Readable output). When NULL, it detects the format on file name extension.
<code>identifications.format</code>	"ibspectra.csv" or "mzid" (PSI MzIdentML format). When NULL, file format is guessed based on extension.
<code>fragment.precision</code>	Fragment precision for extraction of reporter tags: for each tag and spectrum the m/z-intensity pair with it's mass closest to the known reporter tag mass is extracted within the window <code>true_mass +/- fragment.precision/2</code> .
<code>fragment.outlier.prob</code>	Fragment outlier probability filter: After all m/z-intensity pairs have been extracted, those pairs with the <code>fragment.outlier.prob/2</code> most unprecise m/z values are filtered out.
<code>decode.titles</code>	Boolean. Decode spectrum titles in identification file using <code>URLdecode</code> . When extracting the DAT file from Mascot web interface, the spectrum titles are encoded - %20 instead of space, etc. Set <code>decode.titles</code> to TRUE to map these titles to the unescaped MGF titles.
<code>scan.lines</code>	Read files sequentially <code>scan.lines</code> lines at a time. Can help in case of memory issues, set to 10000 or higher, for example.
<code>sep</code>	sep argument of <code>read.table</code>
<code>...</code>	Further arguments handed down to <code>initialize</code> .

Author(s)

Florian P. Breitwieser, Jacques Colinge

See Also

[ProteinGroup](#), [IBSpectra](#), [isobar-preprocessing](#), [isobar-analysis](#), [isobar-plots](#)

Examples

```
data(ibspiked_set1)

# get identifier for Ceruplasmin proteins
ceru.acs <- protein.g(proteinGroup(ibspiked_set1),"CERU")
# create a smaller ibspectra w/ only Ceruplasmins
ib.ceru <- subsetIBSpectra(ibspiked_set1,protein=ceru.acs,direction="include")

# write it to a file
tf <- tempfile("isobar")
write.table(as.data.frame(ib.ceru),sep="\t",file=tf)

# read it again into an IBSpectra object
ib.ceru2 <- readIBSpectra("iTRAQ4plexSpectra",tf,identifications.format="ibspectra")
ib.ceru2

unlink(tf)
```

isobar-plots

IBSpectra plots

Description

Various plots are implement to assure data quality, and accompany preprocessing and analysis.

reporterMassPrecision

`reporterMassPrecision(x)`: Calculates and displays the deviation from the 'true' tag mass - as specified in the IBSpectra object - of each channel.

reporterIntensityPlot

`reporterIntensityPlot(x)`: Displays boxplots of intensity of channels before and after normalization - useful to check the result of normalization.

raplot

`raplot(x, ...)`: Ratio-Absolute intensity plot - will be deprecated by `maplot`

- x IBSpectra object
- ... Parameters to plot function.

plotRatio

`plotRatio(x, channel1, channel2, protein, ...)`: Plots abundances of one protein

x IBSpectra object
channel1
channel2
protein
... Parameters to plot function.

maplot

`maplot(x, channel1, channel2, ...)`: Creates a ratio-versus-intensity plot.

x IBSpectra object.

maplot2

`maplot2()`:

Author(s)

Florian P. Breitwieser, Jacques Colinge

See Also

[IBSpectra](#), [isobar-preprocessing](#) [isobar-analysis](#)

Examples

```
data(ibspiked_set1)
maplot(ibspiked_set1, main="IBSpiked, not normalized")
maplot(normalize(ibspiked_set1), main="IBSpiked, normalized")
```

isobar-preprocessing *IBSpectra preprocessing*

Description

Preprocessing is a necessary step prior to analysis of data. In a sequential order, it is often necessary to correct isotope impurities, to normalize, and subtract additive noise.

Isotope impurity correction

`correctIsotopeImpurities(x)`: Returns impurity corrected IBSpectra object by solving a linear system of equations. See also [isotopeImpurities](#).

Normalization

`normalize(x, f=median, target="intensity", exclude.protein=NULL, use.protein=NULL, f.doapply=TRUE, log=T`

Normalizes the intensities for multiplicative errors. Those changes are most likely produced by pipetting errors, and different hybridization efficiencies, but can also be due to biological reasons. By default, tag intensities are multiplied by a factor so that the median intensity is equal across tags.

f: `f` is applied to each column, unless `f.doapply` is `FALSE`. Then `f` is supposed to compute column-wise statistics of the matrix of intensities. E.g. `colSums` and `colMeans`.

target: One of "intensity" and "ratio".

exclude.proteins Spectra of peptides which might come from these proteins are excluded. Use for example for contaminants and proteins depleted in the experiment.

use.protein: If specified, only spectra coming from this protein are used. Use when a protein is spiked-in as normalization control.

f.isglobal: If true, `f` is applied on each column. If false, `f` is supposed to compute column-wise statistics of the matrix of intensities. E.g. `colSums` and `colMeans`.

log: Used when `target=`ratio.

Subtract additive noise

`subtractAdditiveNoise(x, method="quantile", shared=TRUE, prob=0.01):` method 'quantile' method is supported for now. It take's the prob (0.01) quantile to estimate the noise level. This value is subtracted from all intensities, and all remaining intensities have to be at least that value.

prob See 'method'.

shared If channels are assumed similar in intensity and hence a shared noise level is reasonable. If not, then one level per channel is necessary.

Exclusion of proteins

`exclude(x, proteins.to.exclude):` Removes spectra which are assigned to proteins in `protein.to.exclude` from the object. This can be useful to remove contaminants. It create a new grouping based on the data which is left.

proteins.to.exclude Proteins to exclude.

Author(s)

Florian P. Breitwieser, Jacques Colinge

See Also

[ProteinGroup](#), [IBSpectra](#), [isobar-analysis](#), [isobar-plots](#)

Examples

```
data(ibspiked_set1)
maplot(ibspiked_set1, main="IBSpiked, not normalized")
maplot(normalize(ibspiked_set1), main="IBSpiked, normalized")
```

isobar-reports	<i>Isobar reports</i>
----------------	-----------------------

Description

Generation of LaTeX and XLS reports is helped with functions which facilitate the gathering of relevant information and creation of tikz plots. `create.reports` parses properties (by calling `load.properties`) and initialize environments and computations (by calling `initialize.env`) required by the reports, calls Sweave and pdflatex.

Usage

```
create.reports(properties.file = "properties.R",
               global.properties.file = system.file("report", "properties.R", package = "isobar"),
               args = NULL, ...,
               recreate.properties.env = TRUE, recreate.report.env = TRUE)
```

```
load.properties(properties.file = "properties.R",
                global.properties.file = system.file("report", "properties.R", package="isobar"),
                args = NULL, ...)
```

```
initialize.env(env, properties.env)
```

Arguments

<code>properties.file</code>	File which holds the parameters for data analysis and report generation. It is parsed as R code after the global report configuration file <code>global.properties.file</code> and defines peaklists, identification files, significance levels, etc. See the global properties file for the available options and values.
<code>global.properties.file</code>	<code>system.file("report", "properties.R", package="isobar")</code>
<code>args</code>	Additional (command line) arguments which overrides those in <code>properties.file</code> .
<code>...</code>	Additional properties.
<code>recreate.properties.env</code>	Whether a <code>properties.env</code> existing in the global environment should be used, or it should be recreated.
<code>recreate.report.env</code>	Whether a <code>report.env</code> existing in the global environment should be used, or it should be recreated.
<code>env</code>	Item to be initialized.
<code>properties.env</code>	Environment into which properties are read.

Details

The directory `inst` in the isobar installation directory `system.file("inst", package="isobar")` contains R, Sweave, and LaTeX files as examples of how to create XLS and PDF reports using isobar.

create_reports.R Call with `Rscript`. It is the main file which

1. parses command line options. `--compile` and `--zip` are parsed directly and given as arguments to `create_reports`. Other arguments are given [load.properties](#).
2. calls a perl script to generate a XLS report
3. generates a LaTeX quality control and analysis report

for the XLS report the script `pl/tab2xls.pl` is used, which concatenates CSV files to a XLS. See Perl requirements. Sweave is called on `report/isobar-qc.Rnw` and `report/isobar-analysis.Rnw`. All files are written the working directory.

isobar-qc.Rnw Quality control Sweave file.

isobar-analysis.Rnw Data analysis Sweave file.

properties.R Default configuration for data analysis.

report-utils.tex LaTeX functions for plotting tikz graphics, etc.

Author(s)

Florian P Breitwieser

See Also

[IBSpectra](#), [isobar-preprocessing](#) [isobar-analysis](#)

isobar.data

Isobar Data packages

Description

`ibspiked_set1` and `ibspiked_set2` are objects of class `iTRAQ4plexSpectra`. It contains over 160 protein groups, over 1600 peptides from about 15,000 spectra each, mainly from background proteins and three spiked-in Ceruplasmins (`CERU_HUMAN`, `CERU_MOUSE`, `CERU_RAT`).

Usage

```
data(ibspiked_set1)
data(ibspiked_set2)
data(ib_phospho)
```

Format

`iTRAQ4plexSpectra` objects.

Source

isobar publication. Acquired on Orbitrap instrument w/ 20 offline-fractions and HCD fragmentation.

Examples

```
data(ibspiked_set1)
print(ibspiked_set1)
```

maplot.protein	<i>Ratio intensity plot for individual proteins</i>
----------------	---

Description

Plots ratio-versus-intensity for a selected protein against a reference channel.

Usage

```
maplot.protein(x, relative.to, protein, noise.model = NULL, channels = NULL,
              xlim = NULL, ylim = NULL, identify = FALSE, add = FALSE,
              pchs = NULL, log="xy", legend.pos = "topright", names = NULL,
              legend.cex = 0.8, cols = pchs, ltys = NULL, main = protein,
              xlab = NULL, ylab = NULL, type="ma", ...)
```

Arguments

x	IBSpectra object
relative.to	a character vector specifying reporter tag names. Either of length 1 or same length as channels.
protein	Protein group identifier.
noise.model	NoiseModel object.
channels	Reporter tag names.
xlim	See par.
ylim	See par.
identify	boolean. If true, identify is called with peptide labels.
add	
pchs	a vector of the same length as channels. See pch in plot.default .
log	a character string which contains x if the x axis is to be logarithmic, y if the y axis is to be logarithmic and xy or yx if both axes are to be logarithmic.
legend.pos	see pos in legend .
names	a character string of the same length as channels, legend text.
legend.cex	see cex in legend .
cols	a vector of the same length as channels. See col in plot.default .

ltys	a vector of the same length as channels. See lty in plot.default .
main	a main title for the plot
xlab	a label for the x axis, defaults to a description of x.
ylab	a label for the y axis, defaults to a description of y.
type	type of plot
...	passed to plot .

Author(s)

Florian P. Breitwieser

NoiseModel-class *NoiseModel objects*

Description

A NoiseModel represent the technical variation which is dependent on signal intensity.

Constructor

`new(type, ibspectra, reporterTagNames=NULL, one.to.one=TRUE, min.spectra=10, plot=FALSE, pool=FALSE):`
Creates a new NoiseModel object based on ibspectra object.

`type`: A non-virtual class deriving from NoiseModel: ExponentialNoiseModel, ExponentialNoANoiseModel, InverseNoiseModel, InverseNoANoiseModel

`reporterTagNames`: When NULL, all channels from ibspectra are taken (i.e. `sampleNames(ibspectra)`). Otherwise, specify subset of names

`one.to.one`: Set to false to learn noise model one a non one-to-one dataset

`min.spectra`: When `one.to.one=FALSE`, only take proteins with `min.spectra` to learn noise model.

`plot`: Set to true to plot data the noise model is learnt on.

`pool`: If false, a NoiseModel is estimated on each combination of channels individually, and then the parameters are averaged. If true, the ratios of all channels are pooled and then a NoiseModel is estimated.

Accessor methods

`noiseFunction`: Gets the noise function.

`parameter`: Gets and sets the parameters for the noise function.

`variance`: Gets the variance for data points based on the noise function and parameters.

`stddev`: Convenience function, `sqrt(variance(...))`.

`lowIntensity`: Gets and sets the low intensity slot, denoting the noise region.

`naRegion`: Gets and sets the `na.region` slot.

Examples

```
data(ibspiked_set1)

ceru.proteins <- protein.g(proteinGroup(ibspiked_set1),"CERU")

# normalize
ibspiked_set1 <- normalize(correctIsotopeImpurities(ibspiked_set1))

# remove spiked proteins
ibspiked_set1.noceru <- exclude(ibspiked_set1,ceru.proteins)
ibspiked_set1.justceru <- subsetIBSpectra(ibspiked_set1,protein=ceru.proteins,direction="include")

# learn noise models
nm.i <- new("InverseNoiseModel",ibspiked_set1.noceru)
nm.e <- new("ExponentialNoiseModel",ibspiked_set1.noceru)

#learn on non-one.to.one data: not normalized, with spiked proteins
nm.n <- new("ExponentialNoiseModel",ibspiked_set1.justceru,one.to.one=FALSE)

maplot(ibspiked_set1,noise.model=c(nm.e,nm.i,nm.n),ylim=c(0.1,10))
```

number.ranges

Helper function to transform number lists to ranges

Description

1,2,3,4,5,8,9,10 -> 1-5,8-10

Usage

```
number.ranges(numbers)
```

Arguments

numbers numeric

Value

character

Author(s)

Florian P Breitwieser

Examples

```
number.ranges(c(1,2,3,9,3,10,8,11))
```

observedKnownSites *Observed modification sites.*

Description

Functions to display the modification sites observed for each protein isoform and count the number of modified residues per protein.

Usage

```
observedKnownSites(protein.group, protein.g, ptm.info, modif, modification.name = NULL)

modif.site.count(protein.group, protein.g = reporterProteins(protein.group), modif, take = max)

modif.sites(protein.group, protein.g = reporterProteins(protein.group), modif)
```

Arguments

protein.group	ProteinGroupb object.
protein.g	protein group identifier.
ptm.info	ptm information data.frame, see ?getPtmInfo.
modif	Modification to track, e.g. 'PHOS'.
modification.name	Value to filter 'modification.name' column in ptm.info.
take	should be either max or min: When multiple isoforms are present, which value should be taken for the count?

Author(s)

Florian P. Breitwieser

Examples

```
data(ib_phospho)
data(ptm.info)

# Modification sites of reporter proteins:
# a list of protein groups,
# containing sub-lists of identified sites for each isoform
protein.modif.sites <- sort(modif.site.count(proteinGroup(ib_phospho), modif="PHOS"))

# Details on modification sites of proteins
# detected with most modifications
modif.sites(proteinGroup(ib_phospho), modif="PHOS", protein.g=names(tail(protein.modif.sites)))

# How many sites are known, and how many known sites have been observed?
observedKnownSites(proteinGroup(ib_phospho), modif="PHOS", protein.g=names(tail(protein.modif.sites)), ptm.info=ptm.info)
```

peptide.count	<i>Peptide counts, spectral counts and sequence coverage for Protein-Group objects.</i>
---------------	---

Description

Report the peptide count, spectral count and sequence coverage for supplied proteins.

Usage

```
peptide.count(protein.group, protein.g = reporterProteins(protein.group),
              specificity = c("reporter-specific", "group-specific", "unspecific"), ...)

spectra.count(protein.group, protein.g = reporterProteins(protein.group),
              specificity = c("reporter-specific", "group-specific", "unspecific"),
              modif = NULL, ...)

sequence.coverage(protein.group, protein.g = reporterProteins(protein.group),
                  specificity = c("reporter-specific", "group-specific", "unspecific"),
                  simplify = TRUE, ...)
```

Arguments

protein.group	ProteinGroup object.
protein.g	Protein group identifier.
specificity	Specificity of peptides.
modif	Only count peptides having a certain modification.
simplify	If simplify=TRUE, a named numeric vector is returned, with the mean sequence coverage of the ACs of each protein.g supplied. Else, a list with the length of protein.g is returned having the sequence coverage for each protein AC.
...	Further arguments to peptides

Author(s)

Florian P Breitwieser

See Also

[calculate.emPAI](#), [calculate.dNSAF](#), [ProteinGroup](#)

Examples

```
data(ibspiked_set1)
sc <- spectra.count(proteinGroup(ibspiked_set1))
pc <- peptide.count(proteinGroup(ibspiked_set1))
plot(jitter(sc), jitter(pc), log="xy")
```

 Protein and peptide ratio calculation and summarization

Calculating and Summarizing Protein and Peptide Ratios

Description

A set of functions to create ratios within groups and summarize them. `proteinRatios` serves as hub and calls `combn.matrix`, `combn.protein.tbl` and `summarize.ratios` successively. It can be used to calculate intra-class and inter-class ratios, to assess ratios and variability within and over cases.

Usage

```
proteinRatios(ibspectra, noise.model, reporterTagNames = NULL,
              proteins = reporterProteins(proteinGroup(ibspectra)),
              peptide = NULL, cl = classLabels(ibspectra),
              combn.method = "global", symmetry = FALSE, summarize =
              FALSE, summarize.method = "mult.pval", min.detect =
              NULL, strict.sample.pval = TRUE, strict.ratio.pval =
              TRUE, orient.div = 0, sign.level = 0.05,
              sign.level.rat = sign.level, sign.level.sample =
              sign.level, ratiodistr = NULL, zscore.threshold =
              NULL, variance.function = "maxi", combine = FALSE,
              p.adjust = NULL, reverse = FALSE, cmbn = NULL,
              before.summarize.f = NULL, ...)
```

```
peptideRatiosNotQuant(ibspectra, ..., peptide = unique(fData(ibspectra)[!fData(ibspectra)[["use.for.
peptideRatios(ibspectra, ..., peptide = peptides(proteinGroup(ibspectra), columns = c("peptide", "modi
```

```
combn.matrix(x, method = "global", cl = NULL, vs = NULL)
```

```
combn.protein.tbl(cmbn, reverse = FALSE, ...)
```

```
summarize.ratios(ratios, by.column = "ac", summarize.method = "mult.pval",
                 min.detect = NULL, n.combination = NULL,
                 strict.sample.pval = TRUE, strict.ratio.pval = TRUE,
                 orient.div = 0, sign.level = 0.05, sign.level.rat =
                 sign.level, sign.level.sample = sign.level,
                 variance.function = "maxi", ratiodistr = NULL)
```

Arguments

<code>ibspectra</code>	IBSpectra object
<code>x</code>	for <code>combn.matrix</code> : reporter names. See <code>reporterTagNames</code> . argument of <code>proteinRatios</code> .

<code>ratios</code>	result of <code>combn.protein.tbl</code>
<code>by.column</code>	Column(s) which are the identifiers. Usually 'ac', 'peptide' or <code>c('peptide','modif')</code>
<code>cmbn</code>	result of <code>combn.matrix</code>
<code>before.summarize.f</code>	Function which is called after calculating ratios before summarizing them.
<code>noise.model</code>	NoiseModel for spectra variances
<code>reporterTagName</code>	Reporter tags to use. By default all <code>reporterTagName</code> s of <code>ibspectra</code> object.
<code>proteins</code>	proteins for which ratios are calculated - defaults to all proteins with peptides specific to them.
<code>peptide</code>	peptides for which ratios are calculated.
<code>cl</code>	Class labels. See also <code>?classLabels</code> .
<code>vs</code>	Class label or reporter tag name. When <code>combn.method</code> is "versus.class", all combinations against class <code>vs</code> are computed, when <code>combn.method</code> is "verus.channel", all combinations against channel <code>vs</code> .
<code>combn.method</code>	"global", "interclass", or "intra-class". Defines which ratios are computed, based on class labels <code>cl</code>
<code>method</code>	"global", "interclass", or "intra-class". Defines which ratios are computed, based on class labels <code>cl</code>
<code>symmetry</code>	If true, reports also the inverse ratio
<code>summarize</code>	If true, ratios for each protein are summarized.
<code>summarize.method</code>	"isobar", for now.
<code>min.detect</code>	How many times must a ratio for a protein be present when summarizing? When NULL, defaults to the maximum number of combinations.
<code>strict.sample.pval</code>	If true, missing ratios are penalized by giving them a <code>sample.pval</code> of 0.5.
<code>strict.ratio.pval</code>	If true, take all ratios into account. If false, only take ratios into account which are in the same direction as the majority of ratios
<code>orient.div</code>	Number of ratios which might go in the wrong direction.
<code>sign.level</code>	Significance level
<code>sign.level.rat</code>	Significance level on ratio p-value
<code>sign.level.sample</code>	Significance level on sample p-value
<code>ratiodistr</code>	Protein ratio distribution
<code>variance.function</code>	Variance function
<code>zscore.threshold</code>	z-score threshold to apply
<code>...</code>	Passed to <code>estimateRatio()</code>

combine	If true, a single ratio for all proteins and peptides, resp., is calculated. See estimateRatio .
p.adjust	Set to one of p.adjust.methods to adjust ratio p-values for multiple comparisons. See p.adjust .
reverse	reverse
n.combination	number of combinations possible

Value

'data.frame': 11 variables:

lratio	log ratio
variance	variance
n.spectra	Number of spectra used for quantification
p.value.rat	Signal p-value (NA if ratiodistr is missing)
p.value.sample	Sample p-value (NA if ratiodistr is missing)
is.significant	Is the ratio significant? (NA if ratiodistr is missing)
protein	Protein quantified
r1	r1
r2	r2

Author(s)

Florian P Breitwieser, Jacques Colinge

See Also

[IBSpectra, isobar-preprocessing isobar-analysis](#)

Examples

```
combn.matrix(114:117,method="interclass",cl=as.character(c(1,1,2,2)))
combn.matrix(114:117,method="interclass",cl=as.character(c(1,1,2,2)))
combn.matrix(114:117,method="global")

data(ibspiked_set1)
data(noise.model.hcd)

ceru.proteins <- c("P13635","Q61147")
proteinRatios(ibspiked_set1,noise.model=noise.model.hcd,proteins=ceru.proteins,cl=c("T","T","C","C"),combn.met
```

 ProteinGroup-class *ProteinGroup objects*

Description

The ProteinGroup class is a container for identified peptides and proteins, and groups them to distinguish proteins with specific peptides.

Usage

```
ProteinGroup(from, template=NULL, proteinInfo=data.frame())
```

```
protein.ac(x, protein.g)
```

```
protein.g(x, pattern, variables=c("AC", "name"), ...)
```

Arguments

from	data.frame object to create a ProteinGroup from. See Details from column specifications
template	'template' ProteinGroup object for grouping.
x	ProteinGroup object
protein	character string
proteinInfo	data.frame for proteinInfo slot
protein.g	character string, denoting a 'protein group'.
pattern	character string, see grep for details.
variables	AC maps a protein accession code to a protein group. name maps using protein information from proteinInfo.
...	Passed on to grep .

Details

The ProteinGroup class stores spectrum to peptide to protein mapping.

The proteins are grouped by their evidence, i. e. peptides:

- Peptides with changes only from Leucine to Isoleucine are considered the same, as they cannot be distinguished by MS.
- Proteins which are detected with the same peptides are grouped together to a 'indistinguishable protein' - normally these are splice variants.
- Proteins with specific peptides are 'reporters'.
- Proteins with no specific peptides are grouped under these 'reporters'.

This information is stored in six slots:

spectra.n.peptides a named 'character' vector, names being spectrum identifier and values are peptides.

peptide.n.proteins a 'data.frame' containing the number of proteins the peptides could derive from.

peptide.n.protein a character 'matrix' linking peptides to proteins.

indistinguishable.proteins a 'matrix' contain.

Constructor

ProteinGroup(tbl.prot.pep, template=NULL): Creates a ProteinGroup object.

tbl.prot.pep A 'data.frame' with three columns: 1. Protein, 2. Peptide, 3. Spectrum.

template Optional ProteinGroup object the grouping is based upon.

Coercion

In the code snippets below, x is a ProteinGroup object.

as(from, "ProteinGroup"): Creates a ProteinGroup object from a data.frame.

as.data.frame(x, row.names = NULL, optional = FALSE): Creates a data.frame with columns protein (character), peptide (character), spectrum.

as.concise.data.frame(from): Creates a 'concise' data.frame with one spectrum per row, and protein ACs combined

Accessors

In the following code snippets, x is a ProteinGroup object.

spectrumToPeptide(x): Gets spectrum to peptide assignment.

peptideInfo(x): Peptide information such as protein start position.

peptideSpecificity(x): Gets a 'data.frame' containing the peptide specificity: they can be reporter-specific, group-specific, or non-specific.

peptideNProtein(x): Gets peptide to protein assignment.

indistinguishableProteins(x): Gets the proteins which cannot be distinguished based on peptide evidence.

proteinGroupTable: Gets the protein grouping, listing reporters and group members.

peptides(x, protein=NULL, specificity=c("reporter-specific", "group-specific", "unspecific"), columns="")
Gets all peptides detected, or just those for a protein with the defined specificity. columns might define multiple columns of peptideSpecificity(x). set=union returns the union of peptides of all proteins defined, set=intersect returns the intersection.

Author(s)

Florian P. Breitwieser

See Also

[IBSpectra](#)

Examples

```
tbl <- data.frame(spectrum=1:14,peptide=c(rep(letters[1:3],4),"a","x"),
                 modif=":",start.pos=1,
                 protein=c(rep(c("A","B"),each=6),"C","D"))
pg <- ProteinGroup(tbl)
pg
proteinGroupTable(pg)

data(ibspiked_set1)
pg <- proteinGroup(ibspiked_set1)
ceru.proteins <- protein.g(pg,"CERU")

## all ceru peptides
peptides(pg,ceru.proteins)

## peptides shared by all ceru proteins
peptides(pg,ceru.proteins, set=intersect)
```

proteinInfo-methods *Methods for Function proteinInfo*

Description

proteinInfo slot in ProteinGroup objects contains information about proteins. proteinInfo method allows to get and set it.

getProteinInfoFromUniprot downloads information of contained proteins from Uniprot, getProteinInfoFromBiomart from Biomart.

Usage

```
## S4 method for signature ProteinGroup
proteinInfo(x)

## S4 method for signature ProteinGroup,character,missing
proteinInfo(x, protein.g, select="name", collapse=", ",
            simplify = TRUE, do.warn = TRUE)

## S4 method for signature ProteinGroup,missing,character
proteinInfo(x, protein.ac, select="name", collapse=", ",
            simplify = TRUE, do.warn = TRUE)

proteinInfoIsOnSpliceVariants(protein.info)

# getProteinInfoFromUniprot(x, splice.by = 200, fields = c(accession = "id", name
```

```
#           = "entry%20name", protein_name = "protein%20names",
#           gene_name = "genes", organism = "organism", length =
#           "length", sequence = "sequence"))

getProteinInfoFromNextProt(x)

getProteinInfoFromBiomart(x, database = "Uniprot")

getProteinInfoFromBioDb(x, ..., con = NULL)

getProteinInfoFromEntrez(x, splice.by = 200)
```

Arguments

x	ProteinGroup object
protein.g	Protein group identifier. If supplied, only information for these proteins is returned.
protein.ac	Protein ACs. If supplied, only information for these proteins is returned.
select	indicating columns to select. See Details.
collapse	passed to paste to concatenate information of multiple protein in one protein group.
simplify	If true, a vector or matrix is returned, with the pasted protein information. If false, a list is returned.
do.warn	If true, report diagnostic warning messages.
splice.by	Chunk size for query of Uniprot database.
database	database from which the ACs stem from. Only Uniprot is supported for now.
con	database connection
fields	mapping of CSV field names to proteinInfo field names
...	arguments to build database connection.
protein.info	protein info data.frame

Details

proteinInfo contains columns accession, name, gene_name, protein_name, and possibly length and sequence. accession is mapped with the entry AC is mapped to the entry AC in the database. getProteinInfoFromUniprot is the preferred methods to get the information. getProteinInfoFromBioDb is an example how to implement the query on a local database. Depending on the database, protein information might be available on protein ACs or also on the specific splice variants. This can be queried with the proteinInfoIsOnSpliceVariants function.

See Also

[protein.g](#)

Examples

```
data(ibspiked_set1)
pg <- proteinGroup(ibspiked_set1)

## Not run:
proteinInfo(pg) <- getProteinInfoFromUniprot(pg)
proteinInfo(pg) <- getProteinInfoFromBiomart(pg)

## End(Not run)

proteinInfo(pg,protein.g="P13635")
protein.g(pg,"CERU")
```

proteinNameAndDescription

Get protein gene names and description from protein info of protein group.

Description

Convenience functions to retrieve protein gene names and description for a list of protein group identifiers.

Usage

```
proteinNameAndDescription(protein.group, protein.g = reporterProteins(protein.group), collapse = FALSE)
proteinGeneName(protein.group, protein.g = reporterProteins(protein.group))
proteinDescription(protein.group, protein.g = reporterProteins(protein.group))
proteinID(protein.group, protein.g = reporterProteins(protein.group))
```

Arguments

protein.group ProteinGroup object.
protein.g protein group identifier.
collapse If TRUE, the information for all protein.gs is combined.

Author(s)

Florian P Breitwieser

Examples

```
data(ibspiked_set1)
pg <- proteinGroup(ibspiked_set1)
protein.gs <- protein.g(pg,"CERU")
protein.gs
proteinNameAndDescription(pg,protein.gs)
proteinNameAndDescription(pg,protein.gs,collapse=TRUE)
```

```
proteinGeneName(pg,protein.gs)
proteinDescription(pg,protein.gs)
proteinID(pg,protein.gs)
```

```
ratiosReshapeWide      Reshape output of proteinRatios into wide format
```

Description

Reshape output of proteinRatios into wide format

Usage

```
ratiosReshapeWide(quant.tbl, vs.class = NULL, sep = ".", cmbn = NULL,
                  short.names = FALSE)
```

Arguments

quant.tbl	Output of proteinRatios or peptideRatios.
vs.class	Only return ratios where class1 is vs.class
sep	Separator for column names in the reshape.
cmbn	Not functional.
short.names	If vs.class is set and short.names=TRUE, then the comparison name will be i.e. 'class2' instead of 'class2/class1'.

Author(s)

Florian P. Breitwieser

```
reporter.protein-methods
      Get reporter protein group identifier for protein group identifier
```

Description

Methods for function reporter.protein in package **isobar**

Methods

```
signature(x = "ProteinGroup", protein.g = "character") Get reporter protein for protein group identifier.
```

sanitize	<i>Helper function for LaTeX export</i>
----------	---

Description

Sanitizes strings for LaTeX

Usage

```
sanitize(str, dash = TRUE)
```

Arguments

str	character string to be escaped
dash	should a dash ('-') should be escaped to a '\nobreakdash-'?

Value

escaped character

Author(s)

iQuantitator, Florian P Breitwieser

Examples

```
sanitize("\textbf{123-123}")
```

shared.ratios	<i>Shared ratio calculation</i>
---------------	---------------------------------

Description

Calculate ratios of reporter proteins and subset proteins with shared peptides.

Usage

```
shared.ratios(ibspectra, noise.model, channel1 , channel2 , protein = reporterProteins(proteinGroup(ib
```

Arguments

ibspectra	IBspectra object.
noise.model	NoiseModel object.
channel1	channel1 to compare.
channel2	channel2 to compare.
protein	proteins for which the calculation should be made.
...	Additional arguments passed to estimteRatio.

Value

data.frame

Author(s)

Florian P.\ Breitwieser

See Also

[shared.ratios.sign](#)

`shared.ratios.sign` *Plot and get significantly shared ratios.*

Description

Plot and get significantly shared ratios.

Usage

```
shared.ratios.sign(ress, z.shared, min.spectra = 1, plot = TRUE)
```

Arguments

<code>ress</code>	Result of <code>shared.ratios</code> .
<code>z.shared</code>	<code>z</code> .
<code>min.spectra</code>	Minimal number of spectra needed.
<code>plot</code>	plot.

Author(s)

Florian P.\ Breitwieser

See Also

[shared.ratios](#).

`specificities` *Peptide specificities*

Description

Peptides can appear in multiple proteins and therefore have different specificities.

Details

reporter specific: peptides specific to reporter. group specific: peptides specific to the group. un-specific: peptides shared with other proteins.

spectra.count2 *Spectral count for peptides and proteins in ProteinGroup objects.*

Description

Spectral count for peptides and proteins in ProteinGroup objects. It can - other than [spectra.count](#) - quantify the spectra count on the level of peptides, potentially modified, too,

Usage

```
spectra.count2(ibspectra, value = reporterProteins(protein.group),
               type = "protein.g", specificity = c("reporter-specific", "group-specific", "unspecific"),
               modif = NULL, combine = FALSE, subset = NULL, require.quant = NULL, ...)
```

Arguments

ibspectra	IBSpectra object.
value	List of protein group identifiers or peptides.
type	Either 'protein.g' or 'peptide'.
specificity	Specificity of peptides.
modif	Only count peptides having a certain modification.
combine	If TRUE, only one combined result is returned.
subset	Allows to specify an expression to subset <code>link{featureData}</code> of the <code>ibspectra</code> .
require.quant	If not NULL, it may be 'any' or 'all' to only consider spectra with quantitative information in at least one or all channels.
...	Further arguments to peptides

Author(s)

Florian P Breitwieser

See Also

[spectra.count](#), [ProteinGroup](#)

Examples

```
data(ibspiked_set1)
pg <- proteinGroup(ibspiked_set1)
protein.gs <- protein.g(pg, "CERU")
sc <- spectra.count2(ibspiked_set1, protein.gs)
sc.ik <- spectra.count2(ibspiked_set1, protein.gs, modif="iTRAQ4plex_K")
rbind(spectra.counts=sc, spectra.counts_iTRAQk=sc.ik)
```

subsetIBSpectra *Subset IBSpectra objects*

Description

Returns an IBSpectra object which is a subset of the input, excluding or exclusively containing the peptides or proteins supplied.

Usage

```
subsetIBSpectra(x, protein = NULL, peptide = NULL,  
               direction = "exclude",  
               specificity = c(REPORTERSPECIFIC, GROUPSPECIFIC, UNSPECIFIC), ...)
```

Arguments

x	IBSpectra object.
protein	Protein group identifiers. Use protein.g to get protein group identifiers from protein database ACs.
peptide	Peptide sequences.
direction	either 'include' or 'exclude'.
specificity	When 'protein' is supplied: Which peptides should be selected? See specificities .
...	Further arguments passed to spectrumSel

Author(s)

Florian P Breitwieser

See Also

[protein.g](#), [spectrumSel](#), [specificities](#)

Examples

```
data(ibspiked_set1)  
  
# get Keratin proteins  
keratin.proteins <- protein.g(proteinGroup(ibspiked_set1),"Keratin")  
  
# exclude Keratin proteins  
subsetIBSpectra(ibspiked_set1,protein=keratin.proteins,direction="exclude")
```

Tlsd-class	Class "Tlsd"
------------	--------------

Description

Location scale family T distribution, based on the original T function.

Objects from the Class

Objects can be created by calls of the form `new("Tlsd", df, location, scale)`.

Slots

gaps: Object of class "OptionalMatrix" ~~
 img: Object of class "rSpace" ~~
 param: Object of class "OptionalParameter" ~~
 r: Object of class "function" ~~
 d: Object of class "OptionalFunction" ~~
 p: Object of class "OptionalFunction" ~~
 q: Object of class "OptionalFunction" ~~
 .withSim: Object of class "logical" ~~
 .withArith: Object of class "logical" ~~
 .logExact: Object of class "logical" ~~
 .lowerExact: Object of class "logical" ~~
 Symmetry: Object of class "DistributionSymmetry" ~~

Extends

Class "[AbscontDistribution](#)", directly. Class "[UnivariateDistribution](#)", by class "AbscontDistribution", distance 2. Class "[AcDcLcDistribution](#)", by class "AbscontDistribution", distance 2. Class "[Distribution](#)", by class "AbscontDistribution", distance 3. Class "[UnivDistrListOrDistribution](#)", by class "AbscontDistribution", distance 3.

Methods

No methods defined with class "Tlsd" in the signature.

Author(s)

Florian P. Breitwieser, based on original T distribution class.

Examples

```
showClass("Tlsd")
```

TlsParameter-class *Class "TlsParameter"*

Description

The parameter of a location scale t distribution, used by Tlsd-class

Objects from the Class

Objects can be created by calls of the form `new("TlsParameter", ...)`. Usually an object of this class is not needed on its own, it is generated automatically when an object of the class Tlsd is instantiated.

Slots

df: Object of class "numeric" ~~
location: Object of class "numeric" ~~
scale: Object of class "numeric" ~~
name: Object of class "character" ~~

Extends

Class "[Parameter](#)", directly. Class "[OptionalParameter](#)", by class "Parameter", distance 2.

Methods

No methods defined with class "TlsParameter" in the signature.

Author(s)

Florian P. Breitwieser, based on original TParameter class.

See Also

[Tlsd](#)

Examples

```
showClass("TlsParameter")
```

writeHscoreData *Write identifications into a format suitable for Hscore.*

Description

Write identifications into a format suitable for Hscore.

Usage

```
writeHscoreData(outfile, ids, massfile = "defs.txt")
```

Arguments

outfile	Output file.
ids	IBSpectra identifications data.frame (ie fData).
massfile	Definition file for Hscore.

Author(s)

Florian P. Breitwieser

writeIBSpectra *Write IBSpectra file as CSV in a format readable by readIBSpectra.*

Description

Write IBSpectra file using write.table with defaults in a format readable by readIBSpectra.

Usage

```
writeIBSpectra(ibspectra, file, sep = "\t", row.names = FALSE, ...)
```

Arguments

ibspectra	IBSpectra object
file	file name.
sep	field separator string.
row.names	indicates whether row.names should be written.
...	further arguments to write.table

Author(s)

Florian P Breitwieser

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