

# Package ‘isobar’

July 17, 2025

**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. Features modules for integrating and validating PTM-centric datasets (isobar-PTM). More information on <http://www.ms-isobar.org>.

**Version** 1.55.0

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**biocViews** ImmunoOncology, Proteomics, MassSpectrometry,  
Bioinformatics, MultipleComparisons, QualityControl

**Depends** R (>= 2.10.0), Biobase, stats, methods

**Imports** distr, plyr, biomaRt, ggplot2

**Suggests** MSnbase, OrgMassSpecR, XML, RJSONIO, Hmisc, gplots,  
RColorBrewer, gridExtra, limma, boot, DBI, MASS

**LazyLoad** yes

**License** LGPL-2

**URL** <https://github.com/fbreitwieser/isobar>

**BugReports** <https://github.com/fbreitwieser/isobar/issues>

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IBSpectra-plots.R NoiseModel-class.R Tltd-class.R  
ratio-methods.R distr-methods.R sharedpep-methods.R  
report-utils-xls.R report-utils-tex.R report-utils.R  
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|                |                                                                              |
|----------------|------------------------------------------------------------------------------|
| isobar-package | <i>Analysis and quantitation of isobarically tagged MSMS proteomics data</i> |
|----------------|------------------------------------------------------------------------------|

---

## 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  
 Suggests: MSnbase, XML  
 LazyLoad: yes  
 License: LGPL-2  
 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

## Index:

|                      |                                                             |
|----------------------|-------------------------------------------------------------|
| IBSpectra-class      | IBSpectra objects                                           |
| NoiseModel-class     | NoiseModel objects                                          |
| ProteinGroup-class   | ProteinGroup objects                                        |
| do.log               | Log functions for IBSpectra objects                         |
| fitCauchy            | Fit weighted and unweighted Cauchy and Normal distributions |
| groupMemberPeptides  | Peptide info for protein group members                      |
| human.protein.names  | Info on proteins                                            |
| ibspiked_set1        | Isobar Data packages                                        |
| isobar-analysis      | IBSpectra analysis: Protein and peptide ratio calculation   |
| isobar-import        | Loading data into IBSpectra objects using readIBSpectra     |
| isobar-package       | Analysis and quantitation of isobaric tag Proteomics data   |
| isobar-plots         | IBSpectra plots                                             |
| isobar-preprocessing | IBSpectra preprocessing                                     |
| isobar-reports       | Isobar reports                                              |
| maplot.protein       | MAplot for individual proteins                              |
| number.ranges        | Helper function to transform number lists to ranges         |
| proteinInfo-methods  | Methods for Function proteinInfo                            |
| proteinRatios        | protein and peptide ratios                                  |
| sanitize             | Helper function for LaTeX export                            |

|                    |                                           |
|--------------------|-------------------------------------------|
| shared.ratios      | Shared ratio calculation                  |
| shared.ratios.sign | Plot and get significantly shared ratios. |

Further information is available in the following vignettes:

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

### Author(s)

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

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|                  |                                             |
|------------------|---------------------------------------------|
| calc.delta.score | <i>Calculate Delta Score from Ion Score</i> |
|------------------|---------------------------------------------|

---

### 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

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|                     |                                                                      |
|---------------------|----------------------------------------------------------------------|
| calcPeptidePosition | <i>Recalculate peptide start positions based on protein sequence</i> |
|---------------------|----------------------------------------------------------------------|

---

**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 | <i>Calculate and Adjust Ratio and Sample p-values.</i> |
|-------------------|--------------------------------------------------------|

---

**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, 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 | 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

*emPAI approximate abundance calculations.*

---

**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 <a href="#">Digest</a> .                 |
| ...        | Further arguments to <a href="#">observable.peptides/Digest</a> . |

### 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,
  protein.group.combined, adjust.variance = TRUE,
  correlation = 0, recalculate.pvalue = TRUE)
```



**Arguments**

|                                     |                                                                                 |
|-------------------------------------|---------------------------------------------------------------------------------|
| <code>ibspectra</code>              | IBSpectra object.                                                               |
| <code>peptide.quant.tbl</code>      | Calculated with <code>peptideRatios</code> .                                    |
| <code>protein.quant.tbl</code>      | Calculated with <code>proteinRatios</code> .                                    |
| <code>protein.group.combined</code> | ProteinGroup object generated on both PTM and protein data.                     |
| <code>adjust.variance</code>        | Adjust variance of ratios.                                                      |
| <code>correlation</code>            | Assumed correlation between peptide and protein ratios for variance adjustment. |
| <code>recalculate.pvalue</code>     | Recalculate p-value after variance adjustment.                                  |

**Author(s)**

Florian P. Breitwieser

---

distr-methods

---

*Functions for distribution calculations*


---

**Description**

`calcProbXGreaterThanOrY` calculates the probability that  $X \geq Y$ . `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**

```
calcProbXGreaterThanOrY(X, Y, rel.tol = .Machine$double.eps^0.25, subdivisions = 100L)
calcProbXDiffNormals(X, mu_Y, sd_Y, ..., alternative = c("greater", "less", "two-sided"), progress = FALSE)
#calcCumulativeProbXGreaterThanOrY(Xs, mu_Ys, sd_Ys, alternative = c("greater", "less", "two-sided"), progress = FALSE)
distrprint(X, round.digits = 5)
twodistr.plot(X, Y, n.steps = 1000, min.q = 10^-3)
```

**Arguments**

|                           |                                                                |
|---------------------------|----------------------------------------------------------------|
| <code>X</code>            | Object of the class <code>Distribution</code> .                |
| <code>Y</code>            | Object of the class <code>Distribution</code> .                |
| <code>min.q</code>        | minimum quantile                                               |
| <code>n.steps</code>      | Number of steps.                                               |
| <code>mu_Y</code>         | Numeric vector of parameter <code>mu</code> of a Normal.       |
| <code>sd_Y</code>         | Numeric vector of parameter <code>sd</code> of a Normal.       |
| <code>subdivisions</code> | the maximum number of subintervals                             |
| <code>rel.tol</code>      | relative accuracy requested                                    |
| <code>...</code>          | Additional arguments to <code>calcProbXGreaterThanOrY</code> . |
| <code>alternative</code>  | "less", "greater", or "two-sided".                             |
| <code>progress</code>     | Show text progress bar?                                        |
| <code>round.digits</code> | Round digits for printing.                                     |

**Author(s)**

Florian P. Breitwieser

**Examples**

```
library(distr)
calcProbXGreaterThanOrY(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)
fitTlstd(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 = 7, n.aa.down = 7)
```

**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 <a href="#">IBSpectra</a> 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 <a href="#">readIBSpectra</a> .                                                                                                                                                       |
| 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 | <i>Get PTM site information for identified proteins from public databases.</i> |
|------------|--------------------------------------------------------------------------------|

---

## 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",
                        url.wildcard = "XXX")
```

**Arguments**

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

**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**

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Unported License and is freely available for non-commercial purpose, see <http://www.phosphosite.org/staticDownloads.d>

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[grepl("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 | <i>Info on proteins</i> |
|---------------------|-------------------------|

---

### 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 a 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**

|      |                                                         |
|------|---------------------------------------------------------|
| x    | IBSpectra object                                        |
| name | Name of property to be logged (translates to row name). |
| msg  | 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 = "isobar")

## 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.sam=sign.level,
                      remove.outliers=TRUE,outliers.args=list(method = "iqr", o=0.05,
                                                                method="isobar",fc.threshold=1.3,
                                                                channel1.raw=NULL,channel2.raw=NULL,use.na=FALSE,preweig=1))

## 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 $\text{channel2}/\text{channel1}$ . |
| <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 $\text{channel2}/\text{channel1}$ . |
| <code>protein</code>              | Protein(s) of interest. If present, <code>channel1</code> and <code>channel2</code> must be reporter names. Provide either proteins or peptides.                                     |
| <code>peptide</code>              | Peptide(s) of interest. If present, <code>channel1</code> and <code>channel2</code> 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 <a href="#">specificities</a> .                                                                                                                                                  |
| <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 $1/\sum(1/\text{variances})$ . '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 OUTLIERS function (TODO).                                                                                                                                                                 |
| <code>method</code>            | method taken for ratio computation and selection: one of 'isobar', 'libra', 'multiq', 'pep', 'ttest' and 'compare.all'.                                                                                                      |
| <code>fc.threshold</code>      | When method equals fc, takes this as fold change threshold.                                                                                                                                                                  |
| <code>summarize.f</code>       | A method for summarizing spectrum ratios when no other information is available. For example median or mean.                                                                                                                 |
| <code>channel1.raw</code>      | When given, noise estimation is based on channel1.raw and channel2.raw. These are the intensities of the channels before normalization.                                                                                      |
| <code>channel2.raw</code>      | See channel1.raw.                                                                                                                                                                                                            |
| <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 estimateRatioNumeric 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

type                      Name of class of new IBspectra object: [iTRAQ4plexSpectra](#), [iTRAQ8plexSpectra](#), [TMT2plexSpectra](#), [TMT6plexSpectra](#), or [TMT10plexSpectra](#)

|                                     |                                                                                                                                                                                                                                                                                                                                                                                                             |
|-------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <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>IBpectra</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 <a href="#">URLdecode</a> . 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,quote=FALSE)

# 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=FALSE)`

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.

### Substract 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")
```

### 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

*Ratio intensity plot for individual proteins*


---

**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 = 1, main = protein,
               xlab = NULL, ylab = NULL, type="ma", show.lm = FALSE, ...)
```

**Arguments**

|                          |                                                                                                                                                               |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>x</code>           | IBSpectra object                                                                                                                                              |
| <code>relative.to</code> | a character vector specifying reporter tag names. Either of length 1 or same length as channels.                                                              |
| <code>protein</code>     | Protein group identifier.                                                                                                                                     |
| <code>noise.model</code> | NoiseModel object.                                                                                                                                            |
| <code>channels</code>    | Reporter tag names.                                                                                                                                           |
| <code>xlim</code>        | See <code>par</code> .                                                                                                                                        |
| <code>ylim</code>        | See <code>par</code> .                                                                                                                                        |
| <code>identify</code>    | boolean. If true, <code>identify</code> is called with peptide labels.                                                                                        |
| <code>add</code>         |                                                                                                                                                               |
| <code>pchs</code>        | a vector of the same length as channels. See <code>pch</code> in <a href="#">plot.default</a> .                                                               |
| <code>log</code>         | 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. |
| <code>legend.pos</code>  | see <code>pos</code> in <a href="#">legend</a> .                                                                                                              |
| <code>names</code>       | a character string of the same length as channels, legend text.                                                                                               |
| <code>legend.cex</code>  | see <code>cex</code> in <a href="#">legend</a> .                                                                                                              |
| <code>cols</code>        | a vector of the same length as channels. See <code>col</code> in <a href="#">plot.default</a> .                                                               |
| <code>lty</code>         | a vector of the same length as channels. See <code>lty</code> in <a href="#">plot.default</a> .                                                               |
| <code>main</code>        | a main title for the plot                                                                                                                                     |
| <code>xlab</code>        | a label for the x axis, defaults to a description of x.                                                                                                       |
| <code>ylab</code>        | a label for the y axis, defaults to a description of y.                                                                                                       |
| <code>type</code>        | type of plot                                                                                                                                                  |
| <code>...</code>         | passed to <a href="#">plot</a> .                                                                                                                              |
| <code>show.lm</code>     | show LM                                                                                                                                                       |

**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, or a matrix which defines the desired combination of channels (nrow=2).

**one.to.one:** Set to false to learn noise model on 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.in
```

---

|               |                                                                                         |
|---------------|-----------------------------------------------------------------------------------------|
| 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**

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

**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", combn.vs = NULL,
  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.f
peptideRatios(ibspectra, ..., peptide = peptides(proteinGroup(ibspectra), columns = c("peptide", "

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 c('peptide', 'modif')                                                                                                                                                                   |
| <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>reporterTagNames</code>   | Reporter tags to use. By default all <code>reporterTagNames</code> 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 "versus.channel", all combinations against channel <code>vs</code> . |
| <code>combn.method</code>       | "global", "interclass", "intra-class", "versus.class" or "versus.channel". Defines which ratios are computed, based on class labels <code>cl</code>                                                                                                     |
| <code>method</code>             | See <code>combn.method</code>                                                                                                                                                                                                                           |
| <code>combn.vs</code>           | <code>vs</code> argument for <code>combn</code> , if <code>combn.method</code> is "versus.class" or "versus.channel".                                                                                                                                   |
| <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>                                                                                                   |
| <code>combine</code>            | If true, a single ratio for all proteins and peptides, resp., is calculated. See <a href="#">estimateRatio</a> .                         |
| <code>p.adjust</code>           | Set to one of <code>p.adjust.methods</code> to adjust ratio p-values for multiple comparisons. See <a href="#">p.adjust</a> .            |
| <code>reverse</code>            | reverse                                                                                                                                  |
| <code>n.combination</code>      | number of combinations possible                                                                                                          |

**Value**

'data.frame': 11 variables:

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

```

---

|                    |                             |
|--------------------|-----------------------------|
| ProteinGroup-class | <i>ProteinGroup objects</i> |
|--------------------|-----------------------------|

---

**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 <a href="#">grep</a> for details.                                                    |
| variables   | AC maps a protein accession code to a protein group. name maps using protein information from proteinInfo. |
| ...         | Passed on to <a href="#">grep</a> .                                                                        |

**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 Leucin to Isoleucin 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"), column`

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"))

getProteinInfoFromTheInternet(x)

getProteinInfoFromNextProt(x)

getProteinInfoFromBiomart(x, database = "Uniprot")

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

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

### Arguments

|                           |                                                                                                             |
|---------------------------|-------------------------------------------------------------------------------------------------------------|
| <code>x</code>            | ProteinGroup object                                                                                         |
| <code>protein.g</code>    | Protein group identifier. If supplied, only information for these proteins is returned.                     |
| <code>protein.ac</code>   | Protein ACs. If supplied, only information for these proteins is returned.                                  |
| <code>select</code>       | indicating columns to select. See Details.                                                                  |
| <code>collapse</code>     | passed to <a href="#">paste</a> to concatenate information of multiple protein in one protein group.        |
| <code>simplify</code>     | If true, a vector or matrix is returned, with the pasted protein information. If false, a list is returned. |
| <code>do.warn</code>      | If true, report diagnostic warning messages.                                                                |
| <code>splice.by</code>    | Chunk size for query of Uniprot database.                                                                   |
| <code>database</code>     | database from which the ACs stem from. Only Uniprot is supported for now.                                   |
| <code>con</code>          | database connection                                                                                         |
| <code>fields</code>       | mapping of CSV field names to proteinInfo field names                                                       |
| <code>...</code>          | arguments to build database connection.                                                                     |
| <code>protein.info</code> | 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 = F)
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 | <i>Reshape output of proteinRatios into wide format</i> |
|-------------------|---------------------------------------------------------|

---

### 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 | <i>Get reporter protein group identifier for protein group identifier</i> |
|--------------------------|---------------------------------------------------------------------------|

---

### 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
```

**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 estimateRatio.      |

**Value**

data.frame

**Author(s)**

Florian P\ Breitwieser

**See Also**

[shared.ratios.sign](#)

---

|                    |                                                  |
|--------------------|--------------------------------------------------|
| shared.ratios.sign | <i>Plot and get significantly shared ratios.</i> |
|--------------------|--------------------------------------------------|

---

**Description**

Plot and get significantly shared ratios.

**Usage**

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

**Arguments**

|             |                                   |
|-------------|-----------------------------------|
| ress        | Result of shared.ratios.          |
| z.shared    | z.                                |
| min.spectra | Minimal number of spectra needed. |
| plot        | plot.                             |

**Author(s)**

Florian P\ Breitwieser

**See Also**

[shared.ratios.](#)

---

|               |                              |
|---------------|------------------------------|
| specificities | <i>Peptide specificities</i> |
|---------------|------------------------------|

---

**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 | <i>Spectral count for peptides and proteins in ProteinGroup objects.</i> |
|----------------|--------------------------------------------------------------------------|

---

## 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 <a href="#">expression</a> to subset link{featureData} of the ibspectra.                                 |
| 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 <a href="#">peptides</a>                                                                                 |

## 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 | <i>Subset IBSpectra objects</i> |
|-----------------|---------------------------------|

---

### 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 <a href="#">protein.g</a> 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 <a href="#">specificities</a> .                   |
| ...         | Further arguments passed to <a href="#">spectrumSel</a>                                                              |

### 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 | <i>Write identifications into a format suitable for Hscore.</i> |
|-----------------|-----------------------------------------------------------------|

---

**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 | <i>Write IBSpectra file as CSV in a format readable by readIBSpectra.</i> |
|----------------|---------------------------------------------------------------------------|

---

**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 <a href="#">write.table</a> |

**Author(s)**

Florian P Breitwieser

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