Package 'SWATH2stats'

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Type Package

Title Transform and Filter SWATH Data for Statistical Packages

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Description This package is intended to transform SWATH data from the OpenSWATH software into a format readable by other statistics packages while performing filtering, annotation and FDR estimation.

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Depends R(>= 2.10.0)

Imports data.table, reshape2, grid, ggplot2, stats, grDevices, graphics, utils

Suggests testthat, aLFQ, knitr

Enhances imsbInfer, MSstats

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NeedsCompilation no

VignetteBuilder knitr

R topics documented:

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`SWATH2stats-package` *SWATH2stats*

Description

This package is intended to transform SWATH data from the OpenSWATH software into a format readable by other statistics packages while performing filtering, annotation and FDR assessment.

Details

Package:	SWATH2stats
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Author(s)

Peter Blattmann, Moritz Heusel and Ruedi Aebersold

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References

Blattmann P, Heusel M, Aebersold R. SWATH2stats: An R/Bioconductor Package to Process and Convert Quantitative SWATH-MS Proteomics Data for Downstream Analysis Tools. PLoS ONE 11(4): e0153160 (2016). doi: 10.1371/journal.pone.0153160.

Rost HL, Rosenberger G, Navarro P, Gillet L, Miladinovic SM, Schubert OT, Wolski W, Collins BC, Malmstrom J, Malmstrom L, Aebersold R. OpenSWATH enables automated, targeted analysis of data-independent acquisition MS data. Nature Biotechnology. 2014 Mar;32(3):219-23. doi: 10.1038/nbt.2841.

Choi M, Chang CY, Clough T, Broudy D, Killeen T, MacLean B, Vitek O. MSstats: an R package for statistical analysis of quantitative mass spectrometry-based proteomic experiments.Bioinformatics. 2014 Sep 1;30(17):2524-6. doi: 10.1093/bioinformatics/btu305.

Rosenberger G, Ludwig C, Rost HL, Aebersold R, Malmstrom L. aLFQ: an R-package for estimating absolute protein quantities from label-free LC-MS/MS proteomics data. Bioinformatics. 2014 Sep 1;30(17):2511-3. doi: 10.1093/bioinformatics/btu200.

See Also

aLFQ, MSstats,

`assess_decoy_rate` *assess_decoy_rate: Assess decoy rate*

Description

This function counts the number of decoy peptides.

Usage

```
assess_decoy_rate(data)
```

Arguments

`data`	A data frame that contains at least a column named "FullPeptideName" and "decoy".

Details

A printout is generated to indicate the number of non-decoy, decoy peptides and the rate of decoy vs non-decoy peptides. Unique peptides are counted, so a precursor with different charge states is counted as one peptide. In the column "decoy" the values need to be 1,0 or TRUE and FALSE.

Value

Prints the decoy rate.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data <- OpenSWATH_data
assess_decoy_rate(data)
```

`assess_fdr_byrun` *Assess assay, peptide and protein level FDR by run (for each MS_injection separately) in OpenSWATH output table*

Description

This function estimates the assay, peptide and protein FDR by run in an OpenSWATH result table in dependence of a range of m_score cutoffs. The results can be visualized and summarized by the associated method plot.fdr_table(). It counts target and decoy assays (unique transition_group_id), peptides (unique FullPeptideName) and proteins (unique ProteinName) in the OpenSWATH output table in dependence of m-score cutoff, the useful m_score cutoff range is evaluated for each dataset individually on the fly.

To arrive from decoy counts at an estimation of the false discovery rate (false positives among the targets remaining at a given mscore cutoff) the ratio of false positives to true negatives (decoys) (FFT) must be supplied. It is estimated for each run individually by pyProphet and contained in the pyProphet statistics [Injection_name]_full_stat.csv. As an approximation, the FFTs of multiple runs are averaged and supplied as argument FFT. For further details see the Vignette Section 1.3 and 4.1.

To assess fdr over the entire dataset, please refer to function assess_fdr_overall.

FDR is calculated as FDR = (TN*FFT/T); TN=decoys, T=targets, FFT=see above

Usage

```
assess_fdr_byrun(data, FFT, n.range = 20, output = "pdf_csv", plot = TRUE,
filename = "FDR_report_byrun", output_mscore_levels = c(0.01, 0.001))
```

Arguments

`data`	Annotated OpenSWATH/pyProphet output table. Refer to function sample_annotation from this package for further information.
`FFT`	Ratio of false positives to true negatives, q-values from [Injection_name]_full_stat.csv in pyProphet stats output. As an approximation, the q-values of multiple runs are averaged and supplied as argument FFT. Numeric from 0 to 1. Defaults to 1, the most conservative value (1 Decoy indicates 1 False target).
`n.range`	Option to set the number of magnitude for which the m_score threshold is decreased (e.g. n.range = 10, m-score from 0.1 until 10^-10)^.
`output`	Choose output type. "pdf_csv" creates the output as files in the working directory, "Rconsole" triggers delivery of the output to the console enabling further computation or custom plotting / output.
`plot`	Logical, whether or not to create plots from the results (using the associated method plot.fdr_cube()
`filename`	Optional, modifying the basename of the result files if applicable.
`output_mscore_levels`	Define m-score levels to plot and write the estimated FDR results.

Value

Returns an array of target/decoy identification numbers and calculated FDR values at different m-score cutoffs.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
assess_fdr_byrun(data, FFT=0.7, output = "pdf_csv", plot = TRUE,
filename="Testoutput_assess_fdr_byrun")
```

---

assess_fdr_overall *Assess overall FDR in annotated OpenSWATH/pyProphet output table in dependence of m_score cutoff*

Description

This function estimates the assay, peptide and protein FDR over a multi-run OpenSWATH/pyProphet output table. It counts target and decoy assays (unique transition_group_id), peptides (unique FullPeptideName) and proteins (unique ProteinName) in dependence of the m-score cutoff (1e-2 to 1e-20).

To arrive from decoy counts at an estimation of the false discovery rate (false positives among the targets remaining at a given mscore cutoff) the ratio of false positives to true negatives (decoys) (FFT) must be supplied. It is estimated for each run individually by pyProphet and contained in the pyProphet statistics [Injection_name]_full_stat.csv. As an approximation, the FFTs of multiple runs are averaged and supplied as argument FFT. For further details see the Vignette Section 1.3 and 4.1.

Protein FDR control on peak group quality level is a very strict filter and should be handled with caution.

FDR is calculated as FDR = (TN*FFT/T); TN=decoys, T=targets, FFT=see above

Usage

```
assess_fdr_overall(data, FFT, n.range = 20, output = "pdf_csv", plot = TRUE,
filename="FDR_report_overall")
```

Arguments

data	Data table that is produced by the OpenSWATH/pyProphet workflow
n.range	Option to set the number of magnitude for which the m_score threshold is decreased (e.g. n.range = 10, m-score from 0.1 until 10^-10)^.
FFT	Ratio of false positives to true negatives, q-values from [Injection_name]_full_stat.csv in pyProphet stats output. As an approximation, the q-values of multiple runs are averaged and supplied as argument FFT. Numeric from 0 to 1. Defaults to 1, the most conservative value (1 Decoy indicates 1 False target).

output	Choose output type. "pdf_csv" creates the output as files in the working directory, "Rconsole" triggers delivery of the output to the console enabling further computation or custom plotting / output.
plot	Logical, whether or not to create plots from the results (using the associated method plot.fdr_table()
filename	Optional, modifying the basename of the result files if applicable.

Value

Returns a list of class "fdr_table". If output "pdf_csv" and plot = TRUE were chosen, report files are written to the working folder.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
assess_fdr_overall(data, FFT=0.7, output = "Rconsole", plot = TRUE,
filename="Testoutput_assess_fdr_overall")
```

---

convert4aLFQ *convert4aLFQ: Convert table into the format for aLFQ*

Description

This functions selects the columns necessary for the aLFQ R package.

Usage

```
convert4aLFQ(data, annotation = TRUE)
```

Arguments

data	A data frame containing the SWATH data in transition-level format
annotation	Option to indicate if the data has been annotated, i.e. if the columns Condition, Replicate, Run are present. If option is set to true it will write a new run_id as a string of the combination of these three columns.

Value

Returns a data frame in the appropriate format for aLFQ.

Author(s)

Peter Blattmann

References

Rosenberger G, Ludwig C, Rost HL, Aebersold R, Malmstrom L. aLFQ: an R-package for estimating absolute protein quantities from label-free LC-MS/MS proteomics data. Bioinformatics. 2014 Sep 1;30(17):2511-3. doi: 10.1093/bioinformatics/btu200.

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
raw <- disaggregate(data.filtered.decoy)
data.aLFQ <- convert4aLFQ(raw)
```

`convert4mapDIA` *convert4mapDIA: Convert table into the format for mapDIA*

Description

This functions selects the columns necessary for mapDIA.

Usage

```
convert4mapDIA(data, RT=FALSE)
```

Arguments

`data`	A data frame containing SWATH data.
`RT`	Option to export the retention times.

Value

Returns a data frame in the appropriate format for mapDIA.

Note

The table must not contain any technical replica, the intensity of technical replica is averaged. This function requires the package reshape2.

Author(s)

Peter Blattmann

References

Teo, G., et al. (2015). "mapDIA: Preprocessing and statistical analysis of quantitative proteomics data from data independent acquisition mass spectrometry." J Proteomics 129: 108-120.

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
raw <- disaggregate(data.filtered.decoy)
data.mapDIA <- convert4mapDIA(raw, RT=TRUE)
```

`convert4MSstats` *convert4MSstats: Convert table into the format for MSstats*

Description

This functions selects the columns necessary for MSstats and renames them if necessary.

Usage

```
convert4MSstats(data, replace.values = TRUE, replace.colnames = TRUE,
replace.Unimod = TRUE)
```

Arguments

`data`	A data frame containing SWATH data.
`replace.values`	Option to indicate if negative and 0 values should be replaced with NA.
`replace.colnames`	Option to indicate if column names should be renamed and columns reduced to the necessary columns for MSstats
`replace.Unimod`	Option to indicate if Unimod Identifier should be replaced from ":" to "_".

Details

The necessary columns are selected and three columns renamed: FullPeptideName -> PeptideSequence Charge -> PrecursorCharge align_origfilename -> File

Value

Returns a data frame in the appropriate format for MSstats.

Author(s)

Peter Blattmann

References

Choi M, Chang CY, Clough T, Broudy D, Killeen T, MacLean B, Vitek O. MSstats: an R package for statistical analysis of quantitative mass spectrometry-based proteomic experiments.Bioinformatics. 2014 Sep 1;30(17):2524-6. doi: 10.1093/bioinformatics/btu305.

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
raw <- disaggregate(data.filtered.decoy)
data.mapDIA <- convert4MSstats(raw)
```

`convert4pythonscript` *convert4bashscript: Convert data into the format for running a bash script*

Description

This functions selects the columns suggested to run a python script to change the data from peptide-level to transition-level.

Usage

```
convert4pythonscript(data, replace.Unimod = TRUE)
```

Arguments

`data`	A data frame containing SWATH data.
`replace.Unimod`	Option to indicate if Unimod Identifier should be replaced form ":"" to "_".

Details

The necessary columns are selected and the run column is renamed to align_origfilename for the script. The intensities are taken from the column aggr_Peak_Area and therefore the Intensity column is not exported.

Value

Returns a data frame in the appropriate format to be used by a custom python script stored in the scripts folder.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data,0.01)
data.pythonscript <- convert4pythonscript(data.filtered.decoy)
```

count_analytes *count_analytes: Counts analytes in different injections*

Description

This functions counts the number of different peakgroups, peptides and proteins in different injections

Usage

```
count_analytes(data, column.levels = c("transition_group_id", "FullPeptideName",
"ProteinName"), column.by="run_id", rm.decoy=TRUE)
```

Arguments

data	A data frame containing SWATH data.
column.levels	Columns in which different identifiers should be counted.
column.by	Column for which the different identifiers should be counted for, e.g. for the different injections.
rm.decoy	Option to not remove decoy before counting.

Value

Returns a data frame with the count of the different identifiers per e.g. injection.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
count_analytes(data)
```

disaggregate *disaggregate: Transforms the SWATH data from a peptide- to a transition-level table.*

Description

If the SWATH data should be analyzed on transition-level the data needs to be tranformed from peptide-level table to a transition-level table (one row per transition instead of one row per peptide). The columns "aggr_Fragment_Annotation" and "aggr_Peak_Area" are disaggregated into the new columns "FragmentIon" and "Intensity".

Usage

```
disaggregate(data)
```

Arguments

data	A data frame containing SWATH data.

Value

Returns a data frame containing the SWATH data in a transition-level table.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
raw <- disaggregate(data.filtered.decoy)
```

---

filter_all_peptides *Select all proteins that are supported by peptides.*

Description

This functions counts all proteins that are supported by peptides (including non proteo-typic peptides). All peptides (incl. non proteotypic peptides are selected. For the proteins supproted by proteotypic peptide the "1/" in front of the identifier is removed to facilitate further data processing.

Usage

```
filter_all_peptides(data)
```

Arguments

data	A data frame containing SWATH data.

Value

Returns a data frame with the data from both proteotypic and non-proteotypic peptides.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
data.all <- filter_all_peptides(data.filtered.decoy)
```

filter_mscore *filter_mscore: Filter openSWATH output table according to mscore*

Description

This function filters the SWATH data according to the m_score value, as well as to the number of occurence in the data (requant) and within a condition (condition)

Usage

```
filter_mscore(data, mscore, rm.decoy=TRUE)
filter_mscore_freqobs(data, mscore, percentage=NULL, rm.decoy = TRUE)
filter_mscore_condition(data, mscore, n.replica, rm.decoy = TRUE)
```

Arguments

data	A data frame containing SWATH data.
mscore	Value that defines the mscore threshold according to which the data will be filtered.
n.replica	Number of measurements within at least one condition that have to pass the mscore threshold for this transition.
percentage	Percentage in which replicas the transition has to reach the mscore threshold
rm.decoy	Option to remove the decoys during filtering.

Value

Returns a data frame with the filtered data.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered <- filter_mscore(data, 0.01)
data.filtered <- filter_mscore_freqobs(data, 0.01, 0.8)
data.filtered <- filter_mscore_condition(data, 0.01, 3)
```

`filter_mscore_fdr` *Filter annotated OpenSWATH/pyProphet output table to achieve a high FDR quality data matrix with controlled overall protein FDR and quantitative values for all peptides mapping to these high-confidence proteins (up to a desired overall peptide level FDR quality).*

Description

This function controls the protein FDR over a multi-run OpenSWATH/pyProphet output table and filters all quantitative values to a desired overall/global peptide FDR level.

It first finds a suitable m-score cutoff to minimally achieve a desired global FDR quality on a protein master list based on the function mscore4protfdr. It then finds a suitable m-score cutoff to minimally achieve a desired global FDR quality on peptide level based on the function mscore4pepfdr. Finally, it reports all the peptide quantities derived based on the peptide level cutoff for only those peptides mapping to the protein master list. It further summarizes the protein and peptide numbers remaining after the filtering. It further evaluates the individual run FDR qualities of the peptides (and quantitation events) selected.

Usage

```
filter_mscore_fdr(data, FFT = 1, overall_protein_fdr_target = 0.02,
upper_overall_peptide_fdr_limit = 0.05, rm.decoy = TRUE)
```

Arguments

`data`	Annotated OpenSWATH/pyProphet data table
`FFT`	Ratio of false positives to true negatives, q-values from [Injection_name]_full_stat.csv in pyProphet stats output. As an approximation, the q-values of multiple runs are averaged and supplied as argument FFT. Numeric from 0 to 1. Defaults to 1, the most conservative value (1 Decoy indicates 1 False target). For further details see the Vignette Section 1.3 and 4.1.
`overall_protein_fdr_target`	FDR target for the protein master list for which quantitative values down to the less strict peptide_fdr criterion will be kept/reported. Defaults to 0.02.
`upper_overall_peptide_fdr_limit`	FDR target for the quantitative values kept/reported for all peptides mapping to the high-confidence protein master list. Defaults to 0.05. If all values up to m_score 0.01 shall be kept, set = 1.
`rm.decoy`	Logical T/F, whether decoy entries should be removed after the analysis. Defaults to TRUE. Can be useful to disable to track the influence on decoy fraction by further filtering steps such as requiring 2 peptides per protein.

Value

`data.filtered`	the filtered data frame

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.fdr.filtered<-filter_mscore_fdr(data, FFT=0.7, overall_protein_fdr_target=0.02,
upper_overall_peptide_fdr_limit=0.1)
```

`filter_on_max_peptides` *Filter only for the highest intense peptides*

Description

In order to reduce the data, the data is filtered only for the proteins with the highest intensity peptides.

Usage

```
filter_on_max_peptides(data, n_peptides)
```

Arguments

`data`	A data frame containing SWATH data with the column names: ProteinNames, PeptideSequence, PrecursorCharge, Intensity.
`n_peptides`	Maximum number of highest intense peptides to filter the data on.

Value

Returns a data frame of the filtered data

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered <- filter_mscore_freqobs(data, 0.01,0.8)
data.max <- filter_on_max_peptides(data.filtered, 5)
```

filter_on_min_peptides

Filter openSWATH output for proteins that are identified by a minimum of n independent peptides

Description

This function removes entries mapping to proteins that are identified by less than n_peptides.

Removing single-hit proteins from an analysis can significantly increase the sensitivity under strict protein fdr criteria, as evaluated by e.g. assess_fdr_overall.

Usage

```
filter_on_min_peptides(data, n_peptides)
```

Arguments

data	Data table that is produced by the openSWATH/iPortal workflow.
n_peptides	Number of minimal number of peptide IDs associated with a protein ID in order to be kept in the dataset.

Value

Returns the filtered data frame with only peptides that map to proteins with >= n_peptides peptides.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered <- filter_mscore_freqobs(data, 0.01,0.8)
data.max <- filter_on_max_peptides(data.filtered, 5)
data.min.max <- filter_on_min_peptides(data.max, 3)
```

filter_proteotypic_peptides

Filter for proteins that are supported by proteotypic peptides.

Description

Peptides can match to several proteins. With this function proteotypic peptides, peptides that are only contained in one protein are selected. Additionally the number of proteins are counted and printed.

Usage

```
filter_proteotypic_peptides(data)
```

Arguments

data	A data frame containing SWATH data.

Value

Returns a data frame with only the data supported by proteotypic peptides.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
data.all <- filter_proteotypic_peptides(data.filtered.decoy)
```

---

import_data *import_data: Transforms the column names from a data frame to the required format.*

Description

This functions transforms the column names from a data frame from another format to a data frame with column names used by the OpenSWATH output and required for these functions. During executing of the function the corresponding columns for each column in the data need to be selected. For columns that do not corresond to a certain column 'not applicable' needs to be selected and the column names are not changed.

Usage

```
import_data(data)
```

Arguments

data	A data frame containing the SWATH-MS data (one line per peptide precursor quantified) but with different column names.

Value

Returns the data frame in the appropriate format.

Note

List of column names of the OpenSWATH data:

ProteinName: Unique identifier for protein or proteingroup that the peptide maps to. Proteotypic peptides should be indicated by 1/ in order to be recognized as such by the function filter_proteotypic_peptides.

FullPeptideName: Unique identifier for the peptide.

Charge: Charge of the peptide precursor ion quantified.

Sequence: Naked peptide sequence without modifications.

aggr_Fragment_Annotation: aggregated annotation for the different Fragments quantified for this peptide. In the OpenSWATH results the different annotation in OpenSWATH are concatenated by a semicolon.

aggr_Peak_Area: aggregated Intensity values for the different Fragments quantified for this peptide. In the OpenSWATH results the aggregated Peak Area intensities are concatenated by a semicolon.

transition_group_id: A unique identifier for each transition group used.

decoy: Indicating with 1 or 0 if this transition group is a decoy.

m_score: Column containing the score that is used to estimate FDR or filter. M-score values of identified peak groups are equivalent to a q-value and thus typically are smaller than 0.01, depending on the confidence of identification (the lower the m-score, the higher the confidence).

Column containing the score that is used to estimate FDR or filter.

RT: Column containing the retention time of the quantified peak.

align_origfilename: Column containing the filename or a unique identifier for each injection.

Intensity: column containing the intensity value for each quantified peptide.

Columns needed for FDR estimation and filtering functions: ProteinName, FullPeptideName, transition_group_id, decoy, m_score

Columns needed for conversion to transition-level format (needed for MSStats and mapDIA input): aggr_Fragment_Annotation, aggr_Peak_Area

Author(s)

Peter Blattmann

Examples

```
data('Spyogenes', package = 'SWATH2stats')
head(data)
str(data)
```

`mscore4assayfdr` *Find m_score cutoff to reach a desired FDR on assay level (over the entire OpenSWATH/pyProphet output table)*

Description

This function estimates the m_score cutoff required in a dataset to reach a given overall assay level FDR. It counts target and decoy assays at high resolution across the m_score cutoffs and reports a useful m_score cutoff - assay FDR pair close to the supplied fdr_target level over the entire dataset. The m_score cutoff is returned by the function and can be used in the context of the filtering functions, e.g.:

data.assayFDR1pc<-filter_mscore(data, mscore4assayfdr(data, fdr_target=0.01))

To arrive from decoy counts at an estimation of the false discovery rate (false positives among the targets remaining at a given mscore cutoff) the ratio of false positives to true negatives (decoys) (FFT) must be supplied. It is estimated for each run individually by pyProphet and contained in the pyProphet statistics [Injection_name]_full_stat.csv. As an approximation, the FFTs of multiple runs are averaged and supplied as argument FFT. For further details see the Vignette Section 1.3 and 4.1.

For FDR evaluations on peptide and protein level, please refer to functions mscore4pepfdr mscore4protfdr

Usage

```
mscore4assayfdr(data, FFT = 1, fdr_target = 0.01)
```

Arguments

`data`	Annotated OpenSWATH/pyProphet data table. See function sample_annotation from this package.
`FFT`	Ratio of false positives to true negatives, q-values from [Injection_name]_full_stat.csv in pyProphet stats output. As an approximation, the q-values of multiple runs are averaged and supplied as argument FFT. Numeric from 0 to 1. Defaults to 1, the most conservative value (1 Decoy indicates 1 False target).
`fdr_target`	Assay FDR target, numeric, defaults to 0.01. An m_score cutoff achieving an FDR < fdr_target will be selected. Calculated as FDR = (TN*FFT/T); TN=decoys, T=targets, FFT=see above.

Value

Returns the m_score cutoff selected to arrive at the desired FDR

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
mscore4assayfdr(data, FFT=0.7, fdr_target=0.01)
```

`mscore4pepfdr` *Find m_score cutoff to reach a desired FDR on peptide level (over the entire OpenSWATH/pyProphet output table)*

Description

This function estimates the m_score cutoff required in a dataset to reach a given overall peptide level FDR. It counts target and decoy peptides (unique FullPeptideName) at high resolution across the m_score cutoffs and reports a useful m_score cutoff - peptide FDR pair close to the supplied fdr_target level over the entire dataset. The m_score cutoff is returned by the function and can be used in the context of the filtering functions, e.g.:

data.pepFDR2pc<-filter_mscore(data, mscore4pepfdr(data, fdr_target=0.02))

To arrive from decoy counts at an estimation of the false discovery rate (false positives among the targets remaining at a given mscore cutoff) the ratio of false positives to true negatives (decoys) (FFT) must be supplied. It is estimated for each run individually by pyProphet and contained in the pyProphet statistics [Injection_name]_full_stat.csv. As an approximation, the FFTs of multiple runs are averaged and supplied as argument FFT. For further details see the Vignette Section 1.3 and 4.1.

For FDR evaluations on assay and protein level, please refer to functions mscore4assayfdr mscore4protfdr

Usage

```
mscore4pepfdr(data, FFT = 1, fdr_target = 0.01)
```

Arguments

`data`	Annotated OpenSWATH/pyProphet data table. See function sample_annotation from this package.
`FFT`	Ratio of false positives to true negatives, q-values from [Injection_name]_full_stat.csv in pyProphet stats output. As an approximation, the q-values of multiple runs are averaged and supplied as argument FFT. Numeric from 0 to 1. Defaults to 1, the most conservative value (1 Decoy indicates 1 False target).
`fdr_target`	FDR target, numeric, defaults to 0.01. An m_score cutoff achieving an FDR < fdr_target will be selected. Calculated as FDR = (TN*FFT/T); TN=decoys, T=targets, FFT=see above.

Value

Returns the m_score cutoff selected to arrive at the desired FDR

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
mscore4pepfdr(data, FFT=0.7, fdr_target=0.01)
```

`mscore4protfdr` *Find m_score cutoff to reach a desired FDR on protein level (over the entire OpenSWATH/pyProphet output table)*

Description

This function estimates the m_score cutoff required in a dataset to reach a given overall protein level FDR. This filter is to be used with caution as the resulting quantitative matrix is relatively sparse. It can be filled with quantitative values at a lower FDR quality level. It counts target and decoy peptides (unique ProteinName) at high resolution across the m_score cutoffs and reports a useful m_score cutoff - peptide FDR pair close to the supplied fdr_target level over the entire dataset. The m_score cutoff is returned by the function and can be used in the context of the filtering functions, e.g.:

data.protFDR5pc<-filter_mscore(data, mscore4protfdr(data, fdr_target=0.02))

To arrive from decoy counts at an estimation of the false discovery rate (false positives among the targets remaining at a given mscore cutoff) the ratio of false positives to true negatives (decoys) (FFT) must be supplied. It is estimated for each run individually by pyProphet and contained in the pyProphet statistics [Injection_name]_full_stat.csv. As an approximation, the FFTs of multiple runs are averaged and supplied as argument FFT. For further details see the Vignette Section 1.3 and 4.1.

For FDR evaluations on assay and peptide level, please refer to functions mscore4assayfdr mscore4pepfdr

Usage

```
mscore4protfdr(data, FFT, fdr_target)
```

Arguments

`data`	Annotated OpenSWATH/pyProphet data table. See function sample_annotation from this package.
`FFT`	Ratio of false positives to true negatives, q-values from [Injection_name]_full_stat.csv in pyProphet stats output. As an approximation, the q-values of multiple runs are averaged and supplied as argument FFT. Numeric from 0 to 1. Defaults to 1, the most conservative value (1 Decoy indicates 1 False target).
`fdr_target`	FDR target, numeric, defaults to 0.01. An m_score cutoff achieving an FDR < fdr_target will be selected. Calculated as FDR = (TN*FFT/T); TN=decoys, T=targets, FFT=see above.

Value

Returns the m_score cutoff selected to arrive at the desired FDR quality

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
mscore4protfdr(data, FFT=0.7, fdr_target=0.01)
```

`MSstats_data` *Testing dataset in MSstats format*

Description

A small table with the column names corresponding to the MSstats format. This data is intended only to test functions.

Author(s)

Peter Blattmann

`OpenSWATH_data` *Testing dataset from OpenSWATH*

Description

A small selection of the data obtained from the iPortal pipeline for an experiment with perturbations relating to cholesterol regulation. Protein and Peptides have been anonymized as the data is unpublished.\ The FDR version of the test data contains modified (lowered) decoy peak group m_scores to simulate FDR behaviour of a large dataset.

Author(s)

Peter Blattmann

`plot.fdr_cube` *Plot functionality for FDR assessment result arrays as produced by e.g. the function assess_fdr_byrun()*

Description

This function creates standard plots from result arrays as produced by e.g. the function assess_fdr_byrun(), visualizig assay, peptide and protein level FDR for each run at m-score cutoffs 1e-2 and 1e-3. Furthermore, Target and Decoy ID numbers are visualized.

Usage

```
## S3 method for class 'fdr_cube'
plot(x, output = "Rconsole", filename = "FDR_report_byrun",
plot_mscore_levels = c(0.01, 0.001), ...)
```

Arguments

x	Array of by-run FDR assessment results as produced e.g. by the function assess_fdr_byrun() from this package.
output	Choose output type. "pdf_csv" creates the output as files in the working directory, "Rconsole" triggers delivery of the output to the console enabling further computation and/or custom plotting / output.
filename	Basename for output files to be created (if output = "pdf_csv" has been selected).
plot_mscore_levels	Define m-score levels to plot the estimated FDR results.
...	further arguments passed to method.

Value

Plots in Rconsole or report files.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
x <- assess_fdr_byrun(data, FFT=0.7, output = "Rconsole", plot = FALSE)
plot.fdr_cube(x, output = "pdf_csv", filename = "Assess_fdr_byrun_testplot",
plot_mscore_levels=0.01)
```

---

plot.fdr_table *Plot functionality for results of class "fdr_table" as produced by e.g. the function assess_fdr_overall()*

Description

This function created standard plots from results of class "fdr_table" as produced by e.g. the function assess_fdr_overall() visualizig ID numbers in dependence of estimated FDR and also estimated FDR in dependence of m_score cutoff.

Usage

```
## S3 method for class 'fdr_table'
plot(x, output = "Rconsole", filename = "FDR_report_overall", ...)
```

Arguments

x	List of class "fdr_table" as produced e.g. by the function assess_fdr_overall() from this package.
output	Choose output type. "pdf_csv" creates the output as files in the working directory, "Rconsole" triggers delivery of the output to the console enabling further computation or custom plotting / output.
filename	Basename for output files to be created (if output = "pdf_csv" has been selected).
...	further arguments passed to method.

Value

Plots in Rconsole or report files.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
x <- assess_fdr_overall(data, FFT=0.7, output = "Rconsole", plot = FALSE)
plot.fdr_table(x, output = "pdf_csv", filename = "Assess_fdr_overall_testplot")
```

---

plot_correlation_between_samples

Plots the correlation between injections.

Description

This function plots the Pearson's and Spearman correlation between samples. If decoys are present these are removed before plotting.

Usage

```
plot_correlation_between_samples(data, column.values = "Intensity",
Comparison = transition_group_id ~ Condition + BioReplicate,
fun.aggregate =NULL, label=TRUE, ...)
```

Arguments

`data`	Data frame that is produced by the OpenSWATH/pyProphet workflow
`column.values`	Indicates the columns for which the correlation is assessed. This can be the Intensity or Signal, but also the retention time.
`Comparison`	The comparison for assessing the variability. Default is to assess the variability per transition_group_id over the different Condition and Replicates. Comparison is performed using the dcast() function of the reshape2 package.
`fun.aggregate`	If for the comparison values have to be aggregated one needs to provide the function here.
`label`	Option to print correlation value in the plot.
`...`	further arguments passed to method.

Value

Plots in Rconsole a correlation heatmap and returns the data frame used to do the plotting.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
plot_correlation_between_samples(data)
```

`plot_variation` *Plots the coefficient of variation for different replicates*

Description

This function plots the coefficient of variation within replicates for a given value. If decoys are present these are removed before plotting.

Usage

```
plot_variation(data, column.values = "Intensity",
Comparison = transition_group_id + Condition ~ BioReplicate,
fun.aggregate = NULL, label=TRUE, ...)
```

Arguments

`data`	Data frame that is produced by the OpenSWATH/pyProphet workflow
`column.values`	Indicates the columns for which the variation is assessed. This can be the Intensity or Signal, but also the retention time.
`Comparison`	The comparison for assessing the variability. Default is to assess the variability per transition_group_id and Condition over the different Replicates. Comparison is performed using the dcast() function of the reshape2 package.
`fun.aggregate`	If for the comparison values have to be aggregated one needs to provide the function here.
`label`	Option to print value of median cv.
`...`	further arguments passed to method.

Value

Returns a list with the data and calculated cv and a table that summarizes the mean, median and mode cv per Condition (if Condition is contained in the comparison). In addition it plots in Rconsole a violin plot with the observed coefficient of variations.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
plot_variation(data)
```

plot_variation_vs_total *Plots the total variation versus variation within replicates*

Description

This function plots the total variation and the variation within replicates for a given value. If decoys are present these are removed before plotting.

Usage

```
plot_variation_vs_total(data, column.values = "Intensity",
Comparison1 = transition_group_id  ~ BioReplicate + Condition,
Comparison2 = transition_group_id + Condition ~ BioReplicate,
fun.aggregate = NULL, label=TRUE, ...)
```

Arguments

data	Data table that is produced by the OpenSWATH/pyProphet workflow
column.values	Indicates the columns for which the variation is assessed. This can be the Intensity or Signal, but also the retention time.
Comparison1	The comparison for assessing the total variability. Default is to assess the variability per transition_group_id over the combination of Replicates and different Conditions.
Comparison2	The comparison for assessing the variability within the replicates. Default is to assess the variability per transition_group_id and Condition over the different Replicates.
fun.aggregate	If depending on the comparison values have to be aggregated one needs to provide the function here.
label	Option to print value of median cv.
...	further arguments passed to method.

Value

Plots in Rconsole a violin plot comparing the total variation with the variation within replicates. In addition it returns the data frame from which the plotting is done and a table with the calculated mean, median and mode of the cv for the total or replicate data.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
plot_variation_vs_total(data)
```

`reduce_OpenSWATH_output` *Reduce columns of OpenSWATH data*

Description

This function selects the columns from the standard OpenSWATH output to column needed for MSstats, aLFQ and mapDIA.

Usage

```
reduce_OpenSWATH_output(data, column.names=NULL)
```

Arguments

`data`	A data frame containing SWATH data.
`column.names`	A vector of column names that can be selected.

Value

Returns a data frame with the selected columns.

Note

A basic set of columns are defined in the function and are used if no column names are indicated

Note

The column.names can be omitted and then the following columns are selected that are needed for MSstats and mapDIA analysis: ProteinName, FullPeptideName, Sequence, Charge, aggr_Fragment_Annotation, aggr_Peak_Area, align_origfilename, m_score, decoy, Intensity, RT. This function should be omitted if the data is analyzed afterwards with the aLFQ or imsbInfer package that needs further columns.

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered <- reduce_OpenSWATH_output(data)
```

removeDecoyProteins *Removes decoy proteins from the protein group label*

Description

There exist peptides annotated as protein groups with 2/ProteinA/DECOY_ProteinB. However these are in principal proteotypic peptides and should be annoated 1/ProteinA. This function changes these labels accordingly. The subfunction rmDecoyProt removes the Decoy protein, calling removeDecoyProteins also changes the nubmer before the protein group accordingly.

Usage

```
removeDecoyProteins(data)
```

Arguments

data	A data frame containing SWATH data.

Value

Returns a data frame with changed protein labels.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
data.2 <- removeDecoyProteins(data.filtered.decoy)
```

sample_annotation *sample_annotation: Annotate the SWATH data with the sample information*

Description

For statistical analysis and filtering the measurements need to be annotated with Filename, Condition, BioReplicate, and Run. This functions takes this information from a txt file containing this meta-data.

Usage

```
sample_annotation(data, sample.annotation, data.type="OpenSWATH",
column.file = "align_origfilename", change.run.id = TRUE, verbose=FALSE)
```

Arguments

data	A data frame containing SWATH data.
sample.annotation	A data frame containing the columns: Filename, Condition, BioReplicate, Run. The values contained in the column filename have to be present in the filename of the SWATH data.
data.type	Option to specify the format of the table, if the column names from an OpenSWATH output or MSstats table are used.
column.file	Option to specify the column name where the injection file is specified. Default is set to "align_origfilename".
change.run.id	Option to choose if the run_id column shall be reassigned to a unique value combining the values of Condition, BioReplicate and Run. (Option only possible if data is of format "OpenSWATH")
verbose	Option to turn on reporting on which filename it is working on.

Value

Returns a dataframe with each row annotated for the study design

Author(s)

Peter Blattmann

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
```

Spyogenes *S.pyogenes example data*

Description

A table containing SWATH-MS data from S.pyogenes

Source This table was generated from the original data deposited on PeptideAtlas (PASS00289, file "rawOpenSwathResults_1pcnt_only.tsv") by selecting only the column necessary for the SWATH2stats.

References Rost, H. L., et al. (2014). OpenSWATH enables automated, targeted analysis of data-independent acquisition MS data. Nat Biotechnol 32(3): 219-223.

Study_design *Study design table*

Description

A table containing the meta-data defining the study design.

Filename A unique identifier corresponding to the filename in the SWATH data.

Condition The Condition explains the perturbation performed on this sample.

BioReplicate Number indicating the biological replicate of this sample.

Run A unique number for each MS-injection.

Author(s)

Peter Blattmann

Source

Peter Blattmann

transform_MSstats_OpenSWATH *transform_MSstats_OpenSWATH: Transforms column names to OpenSWATH column names*

Description

This functions transforms the column names from a data frame in MSstats format to a data frame with column names used by the OpenSWATH output. The original table needs to contain at least the 10 columns defined by MSstats: ProteinName, PeptideSequence, PrecursorCharge, FragmentIon, ProductCharge, IsotopeLabelType, Condition, BioReplicate, Run, Intensity.)

Usage

```
transform_MSstats_OpenSWATH(data)
```

Arguments

data	A data frame containing the SWATH data in the MSstats format

Value

Returns the data frame in the appropriate format.

Author(s)

Peter Blattmann

References

Choi M, Chang CY, Clough T, Broudy D, Killeen T, MacLean B, Vitek O. MSstats: an R package for statistical analysis of quantitative mass spectrometry-based proteomic experiments.Bioinformatics. 2014 Sep 1;30(17):2524-6. doi: 10.1093/bioinformatics/btu305.

Examples

```
data("MSstats_data", package="SWATH2stats")
transform_MSstats_OpenSWATH(MSstats_data)
```

`unifyProteinGroupLabels` *Unify the protein group labels*

Description

Unify the protein group labels (2/ProteinA/ProteinB and 2/ProteinB/ProteinA) to one common label (e.g. 2/ProteinA/ProteinB)

Usage

```
unifyProteinGroupLabels(data)
```

Arguments

`data`	A data frame containing SWATH data.

Value

Returns a data frame with the unififed protein labels.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
data.filtered.decoy <- filter_mscore(data, 0.01)
data.unified <- unifyProteinGroupLabels(data.filtered.decoy)
```

write_matrix_peptides *write_matrix_peptides: Writes out an overview matrix of peptides mapping to a FDR quality controlled protein master list at controlled global peptide FDR quality.*

Description

Writes out an overview matrix on peptide level of a supplied (unfiltered or prefiltered) OpenSWATH results data frame. The peptide quantification is achieved by summing the areas under all 6 transitions per precursor and summing all precursors per FullPeptideName. In order to keep the peptide-to-protein association, the FullPeptideName is joined with the ProteinName.

Usage

```
write_matrix_peptides(data, write.csv=FALSE,
filename = "SWATH2stats_overview_matrix_peptidelevel.csv",
rm.decoy = FALSE)
```

Arguments

data	A data frame containing annotated OpenSWATH/pyProphet data.
write.csv	Option to determine if table should be written automatically into csv file.
filename	File base name of the .csv matrix written out to the working folder
rm.decoy	Logical whether decoys will be removed from the data matrix. Defaults to FALSE. It's sometimes useful to know how decoys behave across a dataset and how many you allow into your final table with the current filtering strategy.

Value

No return value, output .csv matrix is written to the working folder.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
write_matrix_peptides(data)
```

write_matrix_proteins *write_matrix_proteins: Writes out an overview matrix of summed signals per protein identifier (lines) over run_id(columns).*

Description

Writes out an overview matrix on protein level of a supplied (unfiltered or filtered) OpenSWATH results data frame. The protein quantification is achieved by summing the areas under all 6 transitions per precursor, summing all precursors per FullPeptideName and all FullPeptideName signals per ProteinName entry.

This function does not select consistently quantified or top peptides but sums all signals availabe that may or may not originate from the same set of peptides across different runs. A more detailed overview can be generated using the function write_matrix_peptides().

Peptide selection can be achieved upstream using e.g. the functions filter_mscore_requant(), filter_on_max_peptides() and filter_on_min_peptides().

Usage

```
write_matrix_proteins(data, write.csv = FALSE,
filename = "SWATH2stats_overview_matrix_proteinlevel.csv",
rm.decoy = FALSE)
```

Arguments

data	A data frame containing annotated OpenSWATH/pyProphet data.
write.csv	Option to determine if table should be written automatically into csv file.
filename	File base name of the .csv matrix written out to the working folder
rm.decoy	Logical whether decoys will be removed from the data matrix. Defaults to FALSE. It's sometimes useful to know how decoys behave across a dataset and how many you allow into your final table with the current filtering strategy.

Value

No return value, output .csv matrix is written to the working folder.

Author(s)

Moritz Heusel

Examples

```
data("OpenSWATH_data", package="SWATH2stats")
data("Study_design", package="SWATH2stats")
data <- sample_annotation(OpenSWATH_data, Study_design)
write_matrix_proteins(data)
```

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