Package 'MQmetrics'

April 10, 2023

Type Package

Title Quality Control of Protemics Data

Version 1.6.0

Description The package MQmetrics (MaxQuant metrics) provides a workflow to analyze the quality and reproducibility of your proteomics mass spectrometry analysis from MaxQuant.Input data are extracted from several MaxQuant output tables and produces a pdf report. It includes several visualization tools to check numerous parameters regarding the quality of the runs. It also includes two functions to visualize the iRT peptides from Biognosys in case they were spiked in the samples.

biocViews Infrastructure, Proteomics, MassSpectrometry, QualityControl, DataImport

License GPL-3

Encoding UTF-8

RoxygenNote 7.1.2

Imports ggplot2, readr, magrittr, dplyr, purrr, reshape2, gridExtra, utils, stringr, ggpubr, stats, cowplot, RColorBrewer, tidyr, scales, grid, rlang, ggforce, grDevices, gtable, plyr, knitr, rmarkdown, ggrepel, gghalves, tools

VignetteBuilder knitr

Suggests testthat (>= 3.0.0), BiocStyle

Config/testthat/edition 3

git_url https://git.bioconductor.org/packages/MQmetrics

git_branch RELEASE_3_16

git_last_commit 1bc9b41

git_last_commit_date 2022-11-01

Date/Publication 2023-04-10

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R topics documented:

`generateReport` *Generates a report including all the plots of MQmetrics.*

Description

Generates a report including all the plots of MQmetrics.

Usage

```
generateReport(
  MQPathCombined,
  output_dir = getwd(),
  name_output_file = "MQmetrics_report.pdf",
  remove_contaminants = TRUE,
  log_base = 2,
  long_names = FALSE,
  sep_names = NULL,
```

```
  intensity_type = "Intensity",
  palette = "Set2",
  UniprotID = NULL,
  segment_width = 1,
  show_shade = TRUE,
  percent_proteins = 0.9,
  show_calibrated_rt = FALSE,
  tolerance = 0.001,
  show_max_value = TRUE,
  peptides_modified = 1,
  show_median = TRUE,
  size_median = 1.5,
  binwidth = 0.1,
  plot_unmodified_peptides = FALSE,
  aggregate_PTMs = TRUE,
  combine_same_residue_ptms = TRUE,
  PTM_of_interest = "Oxidation (M)",
  plots_per_page = 5
)
```

Arguments

`MQPathCombined`	The directory to the "combined" folder where the MaxQuant results are stored.
`output_dir`	The directory where the results will be stored. By default is the working directory.
`name_output_file`	The name of the report generated.
`remove_contaminants`	Whether or not to remove contaminants, reverse and identified by one one peptide.
`log_base`	The logarithmic scale for the intensity. Default is 2.
`long_names`	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
`sep_names`	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
`intensity_type`	The type of intensity of interest. Values: 'Intensity' or 'LFQ'. Default = 'Intensity'.
`palette`	The palette from the Package RColorBrewer. By default is 'Set2'.
`UniprotID`	Uniprot ID of the protein of interest. `PlotProteinCoverage()`.
`segment_width`	Width of the segments to improve visualization. Default is 1. (PlotProteinCoverage).
`show_shade`	Creates a shade showing where the `percent_proteins` are. Default is TRUE. `PlotAllDynamicRange()`,`PlotCombinedDynamicRange()`.
`percent_proteins`	Determines the percentage for the show_shade parameter. Default is 0.90 (90% of the proteins). `PlotAllDynamicRange()`, `PlotCombinedDynamicRange()`.

show_calibrated_rt
: If TRUE, it will also show the calibrated retention time of each iRT peptide. By default = FALSE. `PlotiRT()`.

tolerance
: Error maximum to find the iRT peptides by m/z value. By default is 0.001.

show_max_value
: If TRUE, it will show the max TIC value of each sample. `PlotTotalIonCurrent()`.

peptides_modified
: Minimum number of peptides modified. Default is 5. `PlotPTM()`.

show_median
: If true it will show the median of each group, as a red dashed line.By default is TRUE. `PlotHydrophobicity()`.

size_median
: The width of the median line in the plots.

binwidth
: Selects the binwidth of the histogram. By default = 0.2. `PlotHydrophobicity()`.

plot_unmodified_peptides
: If TRUE, it will show the Unmodified peptides. `PlotPTM()`.

aggregate_PTMs
: If TRUE, same PTM that occur multiple times in the same peptides, will be aggregated together.

combine_same_residue_ptms
: Combine the PTMs that happen in the same residue such as Dimethyl (KR), Trimethyl (KR) into only one group: Methyl (KR).

PTM_of_interest
: Post-Translation Modification of interest. It is important they are defined exactly as MaxQuant does: Examples: 'Oxidation (M)', 'Acetyl (Protein N-term)', 'Unmodified', etc.

plots_per_page
: Establish the maximum number of plots per page.

Value

A pdf document with all the results of MQmetrics package.

Examples

```
## Not run:
MQPathCombined <- system.file('extdata/combined/', package = 'MQmetrics')
generateReport(MQPathCombined)

## End(Not run)
```

---

make_MQCombined *Read MaxQuant Tables From Directory*

Description

Read MaxQuant Tables From Directory

Usage

```
make_MQCombined(MQPathCombined, remove_contaminants = TRUE)
```

Arguments

MQPathCombined	The directory to the "combined" folder where the MaxQuant results are stored.
remove_contaminants	Whether or not to remove contaminants, reverse and identified by one one peptide.

Value

The files from the MaxQuant with the contaminants and Reverse hits removed.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
```

MaxQuantAnalysisInfo *Experiment Information*

Description

Experiment Information

Usage

```
MaxQuantAnalysisInfo(MQCombined)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.

Value

Returns the time in hours:minutes that lasted the whole Experiment.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
MaxQuantAnalysisInfo(MQCombined)
```

PlotAcquisitionCycle *Acquisition Cycle and MS/MS*

Description

Acquisition Cycle and MS/MS

Usage

```
PlotAcquisitionCycle(MQCombined, palette = "Set2", plots_per_page = 5)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.

Value

Two plots per sample, one with the cycle tyme vs retention time, and MS/MS count vs retention time.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotAcquisitionCycle(MQCombined)
```

PlotAllDynamicRange *Plots the dynamic range for all samples*

Description

Plots the dynamic range for all samples

Usage

```
PlotAllDynamicRange(MQCombined, show_shade = TRUE, percent_proteins = 0.9)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
show_shade	Creates a shade showing where the percent_proteins are. Default is TRUE.
percent_proteins	Determines the percentage for the show_shade parameter. Default is 0.90 (90% of the proteins).

Value

Returns one plot for each sample, being the dynamic range.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotAllDynamicRange(MQCombined)
```

PlotAndromedaScore *Andromeda score for the best associated MS/MS spectrum.*

Description

Andromeda score for the best associated MS/MS spectrum.

Usage

```
PlotAndromedaScore(
  MQCombined,
  show_median = TRUE,
  size_median = 1.5,
  palette = "Set2",
  plots_per_page = 5
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
show_median	If true it will show the median of each group, as a red dashed line.By default is TRUE.
size_median	The width of the median line in the plots.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.

Value

Plots the MaxQuant Andromeda Score.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotAndromedaScore(MQCombined)
```

PlotCharge *The charge-state of the precursor ion.*

Description

The charge-state of the precursor ion.

Usage

```
PlotCharge(
  MQCombined,
  palette = "Set2",
  plots_per_page = 5,
  tabular_output = FALSE
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.
tabular_output	If true a table with the information will be the output.

Value

Plots the charge-state of the precursor ion.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotCharge(MQCombined)
```

PlotCombinedDynamicRange *Dynamic range of all the samples combined*

Description

Dynamic range of all the samples combined

Usage

```
PlotCombinedDynamicRange(MQCombined, show_shade = TRUE, percent_proteins = 0.9)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
show_shade	Creates a shade showing where the percent_proteins are. Default is TRUE.
percent_proteins	Determines the percentage for the show_shade parameter. Default is 0.90 (90% of the proteins).

Value

Returns the dynamic range for all samples combined.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotCombinedDynamicRange(MQCombined)
```

PlotHydrophobicity *Peptide hydrophobicity by GRAVY score*

Description

Peptide hydrophobicity by GRAVY score

Usage

```
PlotHydrophobicity(
  MQCombined,
  show_median = TRUE,
  size_median = 1.5,
  binwidth = 0.2,
  palette = "Set2",
  plots_per_page = 5,
  tabular_output = FALSE
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
show_median	If true it will show the median of each group, as a red dashed line.By default is TRUE.
size_median	The width of the median line in the plots.
binwidth	Selects the binwidth of the histogram. By default = 0.2
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.
tabular_output	If true a table with the information will be the output.

Value

Returns a histogram per sample, showing the frequency of the peptide's hydrophobicity GRAVY value.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotHydrophobicity(MQCombined)
```

`PlotIntensity` *Intensity / LFQ intensity per sample.*

Description

Intensity / LFQ intensity per sample.

Usage

```
PlotIntensity(
  MQCombined,
  split_violin_intensity = TRUE,
  intensity_type = "Intensity",
  log_base = 2,
  long_names = FALSE,
  sep_names = NULL,
  palette = "Set2"
)
```

Arguments

`MQCombined`	Object list containing all the files from the MaxQuant output. It is the result from using `make_MQCombined`.
`split_violin_intensity`	If TRUE, both the LFQ and the Intensity will be shown in the same plot. If FALSE, it can be specified in the intensity_type which intensity to visualize.
`intensity_type`	The type of intensity. Values: 'Intensity' or 'LFQ'. Only useful if split_violin_intensity = FALSE. Default is Intensity.
`log_base`	The logarithmic scale for the intensity. Default is 2.
`long_names`	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
`sep_names`	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
`palette`	The palette from the Package RColorBrewer. By default is 'Set2'.

Value

A violin plot and boxplot of the intensities in each sample.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotIntensity(MQCombined)
```

PlotiRT *Max intensities of the iRT peptides in each sample.*

Description

Max intensities of the iRT peptides in each sample.

Usage

```
PlotiRT(
  MQCombined,
  show_calibrated_rt = FALSE,
  tolerance = 0.001,
  plots_per_page = 5
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
show_calibrated_rt	If TRUE, it will also show the calibrated retention time of each iRT peptide. By default = FALSE.
tolerance	Error maximum to find the iRT peptides by m/z value. by default is 0.001.
plots_per_page	Establish the maximum number of plots per page.

Value

A plot showing the iRT peptide in each sample vs the Retention time.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotiRT(MQCombined)
```

PlotiRTScore *Score vs retention time of the iRT peptides*

Description

Score vs retention time of the iRT peptides

Usage

```
PlotiRTScore(MQCombined, tolerance = 0.001, plots_per_page = 5)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
tolerance	Error maximum to find the iRT peptides by m/z value. by default is 0.001.
plots_per_page	Establish the maximum number of plots per page.#'

Value

A plot for each sample showing a linear regression of the iRT peptides' retention time vs the score.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotiRT(MQCombined)
```

PlotIsotopePattern *Plot Isotope Pattern and Isotope Pattern Sequenced*

Description

Plot Isotope Pattern and Isotope Pattern Sequenced

Usage

```
PlotIsotopePattern(
  MQCombined,
  long_names = FALSE,
  sep_names = NULL,
  position_dodge_width = 1,
  palette = "Set2"
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
long_names	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
sep_names	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
position_dodge_width	Position of the columns within each others.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.

Value

Returns a plot Isotope Pattern and Isotope Pattern Sequenced.

Examples

```
MQPathCombined <- system.file('extdata/combined/', package = 'MQmetrics')
MQCombined <- make_MQCombined(MQPathCombined)
PlotIsotopePattern(MQCombined)
```

PlotMsMs *Comparison of the MS/MS submitted and identified in each sample.*

Description

Comparison of the MS/MS submitted and identified in each sample.

Usage

```
PlotMsMs(
  MQCombined,
  long_names = FALSE,
  sep_names = NULL,
  position_dodge_width = 1,
  palette = "Set2"
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
long_names	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.

sep_names	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
position_dodge_width	Position of the columns within each others.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.

Value

Plots the MS/MS submitted and Identified in each sample.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotMsMs(MQCombined)
```

PlotPCA *Principal Component Analysis of the Intensity values.*

Description

Principal Component Analysis of the Intensity values.

Usage

```
PlotPCA(MQCombined, intensity_type = "Intensity", palette = "Set2")
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
intensity_type	The type of intensity. Values: 'Intensity' or 'LFQ'.
palette	The palette from the Package RColorBrewer. By default is 'Set2'. Default is Intensity.

Value

A PCA plot of the Intesities of all the samples.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotPCA(MQCombined)
```

PlotPeaks *Total number of peaks detected and sequenced*

Description

Total number of peaks detected and sequenced

Usage

```
PlotPeaks(
  MQCombined,
  long_names = FALSE,
  sep_names = NULL,
  position_dodge_width = 1,
  palette = "Set2"
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
long_names	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
sep_names	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
position_dodge_width	Position of the columns within each others.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.

Value

Plots the total number of peaks detected in the full scans and the total number of peaks sequenced by tandem MS.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotPeaks(MQCombined)
```

PlotPeptidesIdentified *Total number of peaks detected and sequenced*

Description

Total number of peaks detected and sequenced

Usage

```
PlotPeptidesIdentified(
  MQCombined,
  long_names = FALSE,
  sep_names = NULL,
  palette = "Set2"
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
long_names	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
sep_names	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.

Value

Plots the total number of unique peptide amino acid sequences identified from the recorded tandem mass spectra.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotPeptidesIdentified(MQCombined)
```

PlotProteaseSpecificity *Protease Specificity*

Description

Protease Specificity

Usage

```
PlotProteaseSpecificity(
  MQCombined,
  palette = "Set2",
  plots_per_page = 5,
  tabular_output = FALSE
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.
tabular_output	If true a table with the information will be the output.

Value

Two plots per sample: Peptide length distribution and the number of missed enzymatic cleavages.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotProteaseSpecificity(MQCombined)
```

PlotProteinCoverage *Protein coverage and degradation.*

Description

Protein coverage and degradation.

Usage

```
PlotProteinCoverage(
  MQCombined,
  UniprotID = NULL,
  log_base = 2,
  segment_width = 2,
  palette = "Set2",
  plots_per_page = 5
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
UniprotID	Uniprot ID of the protein of interest.
log_base	The logarithmic scale for the intensity. Default is 2.
segment_width	Width of the segments to improve visualization. Default is 1.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.

Value

Two plots for each sample, the end position vs the start position of each peptide of the given protein found. And the Intensity of a given peptide and its length.

Examples

```
MQPathCombined <- system.file('extdata/combined/', package = 'MQmetrics')
MQCombined <- make_MQCombined(MQPathCombined)
PlotProteinCoverage(MQCombined, UniprotID = 'Q15149')
```

PlotProteinOverlap *Protein Overlap Between Samples*

Description

Protein Overlap Between Samples

Usage

```
PlotProteinOverlap(MQCombined, tabular_output = FALSE)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
tabular_output	If true a table with the information will be the output.

Value

A plot showing the protein coverage in all samples.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotProteinOverlap(MQCombined)
```

PlotProteinPeptideRatio

Identification Ratio Between Peptides and Proteins

Description

Identification Ratio Between Peptides and Proteins

Usage

```
PlotProteinPeptideRatio(
  MQCombined,
  intensity_type = "Intensity",
  long_names = FALSE,
  sep_names = NULL
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
intensity_type	The type of intensity of interest. Values: 'Intensity' or 'LFQ'. Default = 'Intensity'.
long_names	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
sep_names	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.

Value

Returns one plot showing the proteins identified vs the peptide/protein ratio in each experiment.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotProteinPeptideRatio(MQCombined)
```

`PlotProteinsIdentified` *Proteins Identified per sample.*

Description

Proteins Identified per sample.

Usage

```
PlotProteinsIdentified(
  MQCombined,
  intensity_type = "Intensity",
  long_names = FALSE,
  sep_names = NULL,
  palette = "Set2"
)
```

Arguments

`MQCombined`	Object list containing all the files from the MaxQuant output. It is the result from using `make_MQCombined`.
`intensity_type`	The type of intensity. Values: 'Intensity' or 'LFQ'. Only useful if split_violin_intensity = FALSE. Default is Intensity.
`long_names`	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
`sep_names`	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
`palette`	The palette from the Package RColorBrewer. By default is 'Set2'.

Value

A plot showing the number of proteins identified per sample and the number of missing values.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotProteinsIdentified(MQCombined)
```

PlotPTM *Post-Translational Modifications*

Description

Post-Translational Modifications

Usage

```
PlotPTM(
  MQCombined,
  peptides_modified = 1,
  plot_unmodified_peptides = FALSE,
  log_base = 2,
  aggregate_PTMs = TRUE,
  combine_same_residue_ptms = TRUE,
  palette = "Set2",
  plots_per_page = 5
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
peptides_modified	Minimum number of peptides modified. Default is 5.
plot_unmodified_peptides	If TRUE, it will show the Unmodified peptides.
log_base	The logarithmic scale for the intensity. Default is 2.
aggregate_PTMs	If TRUE, same PTM that occur multiple times in the same peptides, will be aggregated together.
combine_same_residue_ptms	Combine the PTMs that happen in the same residue such as Dimethyl (KR), Trimethyl (KR) into only one group: Methyl (KR).
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.

Value

Two plots per sample

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotPTM(MQCombined)
```

`PlotPTMAcrossSamples` *Plot PTM across samples*

Description

Plot PTM across samples

Usage

```
PlotPTMAcrossSamples(
  MQCombined,
  PTM_of_interest = "Oxidation (M)",
  log_base = 2,
  long_names = FALSE,
  sep_names = NULL
)
```

Arguments

`MQCombined`	Object list containing all the files from the MaxQuant output. It is the result from using `make_MQCombined`.
`PTM_of_interest`	Post-Translation Modification of interest. It is important they are defined exactly as MaxQuant does: Examples: 'Oxidation (M)', 'Acetyl (Protein N-term)', 'Unmodified', etc.
`log_base`	The logarithmic scale for the intensity. Default is 2.
`long_names`	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
`sep_names`	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.

Value

A plot showing the PTM of interest.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotPTMAcrossSamples(MQCombined, PTM_of_interest = 'Oxidation (M)')
```

PlotTotalIonCurrent *Total Ion Current*

Description

Total Ion Current

Usage

```
PlotTotalIonCurrent(
  MQCombined,
  show_max_value = TRUE,
  palette = "Set2",
  plots_per_page = 5
)
```

Arguments

MQCombined	Object list containing all the files from the MaxQuant output. It is the result from using make_MQCombined.
show_max_value	If TRUE, it will show the max TIC value of each sample.
palette	The palette from the Package RColorBrewer. By default is 'Set2'.
plots_per_page	Establish the maximum number of plots per page.

Value

Returns a plot the Total Ion Current in each sample. The maximum value is also plotted.

Examples

```
MQPathCombined <- system.file("extdata/combined/", package = "MQmetrics")
MQCombined <- make_MQCombined(MQPathCombined)
PlotTotalIonCurrent(MQCombined)
```

ReportTables *Report Tables with summary data*

Description

Report Tables with summary data

Usage

```
ReportTables(
  MQCombined,
  long_names = FALSE,
  sep_names = NULL,
  log_base = 2,
  intensity_type = "Intensity"
)
```

Arguments

MQCombined	The directory to the "combined" folder where the MaxQuant results are stored.
long_names	If TRUE, samples having long names will be considered, and the name will be split by sep_names. By default = FALSE.
sep_names	If long_names is TRUE, sep_names has to be selected. Samples names will be split. By default is NULL.
log_base	The logarithmic scale for the intensity. Default is 2.
intensity_type	The type of intensity. Values: 'Intensity' or 'LFQ'.

Value

A list with four tables are generated: - Protein Information - Intensity Information - Peptide Charge Information - Peptide hydrophobicity Information

Examples

```
MQPathCombined <- system.file('extdata/combined/', package = 'MQmetrics')
MQCombined <- make_MQCombined(MQPathCombined)
ReportTables(MQCombined)
```

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