

Package ‘MQmetrics’

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Type Package

Title Quality Control of Proteomics Data

Version 1.4.0

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.

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License GPL-3

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generateReport	<i>Generates a report including all the plots of MQmetrics.</i>
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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 time 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	<i>Intensity / LFQ intensity per sample.</i>
---------------	--

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 Intensities of all the samples.

Examples

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

PlotPeaks	<i>Total number of peaks detected and sequenced</i>
-----------	---

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 <code>make_MQCombined</code> .
long_names	If TRUE, samples having long names will be considered, and the name will be split by <code>sep_names</code> . By default = FALSE.
sep_names	If <code>long_names</code> is TRUE, <code>sep_names</code> 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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