

# Package ‘MQmetrics’

April 12, 2022

**Type** Package

**Title** Quality Control of Proteomics Data

**Version** 1.2.0

**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, ggridges,  
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\_14

**git\_last\_commit** ba5d543

**git\_last\_commit\_date** 2021-10-26

**Date/Publication** 2022-04-12

**Author** Alvaro Sanchez-Villalba [aut, cre],  
Thomas Stehrer [aut],  
Marek Vrbacky [aut]

**Maintainer** Alvaro Sanchez-Villalba <[sanchezvillalba.alvaro@gmail.com](mailto:sanchezvillalba.alvaro@gmail.com)>

**R topics documented:**

generateReport . . . . .	2
make_MQCombined . . . . .	4
MaxQuantAnalysisInfo . . . . .	5
PlotAcquisitionCycle . . . . .	6
PlotAllDynamicRange . . . . .	6
PlotAndromedaScore . . . . .	7
PlotCharge . . . . .	8
PlotCombinedDynamicRange . . . . .	8
PlotHydrophobicity . . . . .	9
PlotIntensity . . . . .	10
PlotiRT . . . . .	11
PlotiRTScore . . . . .	12
PlotIsotopePattern . . . . .	12
PlotMsMs . . . . .	13
PlotPCA . . . . .	14
PlotPeaks . . . . .	15
PlotPeptidesIdentified . . . . .	16
PlotProteaseSpecificity . . . . .	17
PlotProteinCoverage . . . . .	17
PlotProteinOverlap . . . . .	18
PlotProteinPeptideRatio . . . . .	19
PlotProteinsIdentified . . . . .	20
PlotPTM . . . . .	21
PlotPTMAcrossSamples . . . . .	22
PlotTotalIonCurrent . . . . .	23
ReportTables . . . . .	23
<b>Index</b>	<b>25</b>

---

generateReport	<i>Generates a report including all the plots of MQmetrics.</i>
----------------	---

---

**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	<i>Andromeda score for the best associated MS/MS spectrum.</i>
--------------------	--

---

**Description**

Andromeda score for the best associated MS/MS spectrum.

**Usage**

```
PlotAndromedaScore(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**

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)
```



# Index

[generateReport](#), 2

[make\\_MQCombined](#), 4

[MaxQuantAnalysisInfo](#), 5

[PlotAcquisitionCycle](#), 6

[PlotAllDynamicRange](#), 6

[PlotAndromedaScore](#), 7

[PlotCharge](#), 8

[PlotCombinedDynamicRange](#), 8

[PlotHydrophobicity](#), 9

[PlotIntensity](#), 10

[PlotiRT](#), 11

[PlotiRTScore](#), 12

[PlotIsotopePattern](#), 12

[PlotMsMs](#), 13

[PlotPCA](#), 14

[PlotPeaks](#), 15

[PlotPeptidesIdentified](#), 16

[PlotProteaseSpecificity](#), 17

[PlotProteinCoverage](#), 17

[PlotProteinOverlap](#), 18

[PlotProteinPeptideRatio](#), 19

[PlotProteinsIdentified](#), 20

[PlotPTM](#), 21

[PlotPTMAcrossSamples](#), 22

[PlotTotalIonCurrent](#), 23

[ReportTables](#), 23