

# Package ‘MACSQuantifyR’

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**Type** Package

**Title** Fast treatment of MACSQuantify FACS data

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**Description** Automatically process the metadata of MACSQuantify FACS sorter.

It runs multiple modules: i) imports of raw file and graphical selection of duplicates in well plate, ii) computes statistics on data and iii) can compute combination index.

**Imports** readxl, graphics, tools, utils, grDevices, ggplot2, ggrepel, methods, stats, latticeExtra, lattice, rmarkdown, png, grid, gridExtra, prettydoc, rvest, xml2

**biocViews** DataImport, Preprocessing, Normalization, FlowCytometry, DataRepresentation, GUI

**License** Artistic-2.0

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 7.1.0

**Suggests** knitr, testthat, R.utils, spelling

**VignetteBuilder** knitr

**Language** en-US

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barplot_data	<i>Generate barplots</i>
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### Description

Uses the informations stored in the statistic tables of the MACSQuant object to generate barplots for the specified conditions. Plots can also be saved in the form of a png file in the output\_MQ directory.

### Usage

```
barplot_data(MACSQuant,plt.col=NULL,plt.conditions=NULL, plt.flavour=NULL,
plt.labels = NULL, plt.combo=FALSE,plt.3D.only = NULL,...)
```

### Arguments

MACSQuant	object of class MACSQuant resulting of the function load_maxQuant(). Contains the original data table
plt.col	In case of manual run is used to define the bar colors. (must be the same for all conditions)
plt.conditions	user defined vector of conditions to plot (example: plt.conditions=c(1:9))
plt.flavour	Which barplot to produce, cell count or percentage of fluorochrome (i.e: "counts","percent")
plt.labels	xlabels of the plot
plt.combo	Does the experiment involves multiple variables (i.e some condition are a drug combination screening)
plt.3D.only	Whether to plot 3D barplot alone
...	params for lattice cloud namely z and x for parameter screen default for z and x are c(-110,-70) and argument xlab and ylab

**Value**

returns a barplot of the data

**Examples**

```
drugs_R_image <- system.file("extdata",
  "drugs.RDS",
  package = "MACSQuantifyR")
MACSQuant <- readRDS(drugs_R_image)
flavour <- "counts"
number_of_conditions <-
  slot(MACSQuant, "param.experiment")$number_of_conditions
plt.col <- c(rep(2, number_of_conditions), 1)
barplot_data(MACSQuant,
  plt.col = plt.col,
  plt.conditions = NULL,
  plt.flavour = flavour,
  plt.labels = NULL,
  plt.combo = FALSE)
```

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combination\_index      *compute combination index*

---

**Description**

This function allows the user to compute combination index on the drug combinations. This function also generates intermediary plots and tables.

**Usage**

```
combination_index(MACSQuant, ...)
```

**Arguments**

MACSQuant	object of class MACSQuant resulting of the function load_maxQuant(). Contains the original data table
...	params for lattice cloud namely z and x for parameter screen default for z and x are c(-110,-70) and argument xlab and ylab

**Value**

Several plots and combination index

**References**

Chou, T. C. (2006). Theoretical basis, experimental design, and computerized simulation of synergism and antagonism in drug combination studies. *Pharmacological reviews*, 58(3), 621-681.

**Examples**

```

filepath <- system.file("extdata", "drugs.Rdata",
  package = "MACSQuantifyR")
load(filepath)
combination_index(MACSQuant)

```

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generate_report	<i>Word report generation</i>
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**Description**

Allows the user to generate a report at every steps of the analysis  
 Also generates a complete report with the graphics

**Usage**

```
generate_report(MACSQuant)
```

**Arguments**

MACSQuant	object of class MACSQuant resulting of the function load_maxQuant(). Contains the original data table
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**Value**

A formatted report

**Examples**

```

drugs_R_image <- system.file("extdata",
  "drugs.RDS",
  package = "MACSQuantifyR")
MACSQuant <- readRDS(drugs_R_image)
generate_report(MACSQuant)

```

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load_MACSQuant	<i>Load xls file from maxQuant 96-well-plate device</i>
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**Description**

Load xls file from maxQuant 96-well-plate device

**Usage**

```
load_MACSQuant(filepath, sheet_name= NULL, MACSQuant.obj= NULL)
```

**Arguments**

filepath	path of the excel file
sheet_name	Name of the sheet to load (optional, first sheet is default)
MACSQuant.obj	object of class MACSQuant

**Value**

An object called MACSQuant of class MACSQuant containing variable my\_data that corresponds to the data of the excel file in R

**Examples**

```
filepath <- system.file("extdata", "SingleDrugs.xlsx",  
  package = "MACSQuantifyR")  
# load_MACSQuant(filepath)
```

---

MACSQuant

*The MACSQuant Class*

---

**Description**

MACSQuant object contains all the data and the user parameters

**Slots**

my\_data Contains the raw data

my\_data\_sorted Contains the sorted data (according to replicates order)

my\_replicates\_sorted Contains the sorted matrix containing replicates names

experiment\_name Contains the experiment name given by the user

statistics Contains the statistics for each condition

combination.index.df data.frame that contains the outputs of the combination\_index function

param.experiment list that contains the parameters relative to the experiment (i.e, number of replicates, number of conditions...)

param.output List that contains the parameters relative to the report generation and outputs (i.e, save intermediary results, generate full report..)

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new\_class\_MQ                      *Create a new MACSQuant object*

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### Description

The user can create a new custom MACSQuant object This function is also used in internal code for MACSQuant initialization

### Usage

```
#initialize empty MACSQuant object
new_class_MQ(my_data=NULL,my_data_sorted=NULL,my_replicates_sorted=NULL,
experiment_name=NULL,statistics=NULL,combination.index.df=NULL,
number_of_replicates=NULL,number_of_conditions=NULL,doses=NULL,
doses.alt=NULL,c_names=NULL, control=NULL,plt.title=NULL,
plt.labels=NULL,plt.col=NULL,save.files=NULL,path=tempdir())
#initialize custom MACSQuant object
new_class_MQ(my_data,my_data_sorted=NULL,my_replicates_sorted=NULL,
experiment_name=NULL,statistics=NULL,combination.index.df=NULL,
number_of_replicates=NULL,number_of_conditions=NULL,
doses=NULL,doses.alt=NULL, c_names=NULL,control=NULL,plt.title=NULL,
plt.labels=NULL,plt.col=NULL, save.files=NULL,path=tempdir())
```

### Arguments

my_data	Contains the raw data
my_data_sorted	Contains the sorted data (according to replicates order)
my_replicates_sorted	Contains the sorted matrix containing replicates names
experiment_name	User defined experiment named. Used for the report generation
statistics	Contains the statistics for each condition
combination.index.df	data.frame that contains the outputs of the combination_index function
number_of_replicates	For each condition, the number of duplicates (must be the same for all conditions)
number_of_conditions	The number of conditions tested (eg: Drug 1 alone, Drug 2 alone)
doses	Numeric vector representing doses for each conditions
doses.alt	In case of interaction test second dose vector
c_names	Vector containing experiment names
control	logical: is there a control in this experiment (eg: Staurosporin)
plt.title	Title of the experiment to add to the barplot

plt.labels	legend labels for the bar plot
plt.col	color vector for the graphical representations
save.files	Used to save the image in the output folder
path	path of the experiment output folder (default '.')

**Value**

A formatted report file along with intermediates results

**Examples**

```
# initialize empty MACSQuant object
new_class_MQ()
# initialize custom MACSQuant object
my_data <- data.frame(character(length = 10), character(length = 10),
  numeric(length = 10), numeric(length = 10))
names(my_data) <- c("Full path", "WID", "%-#", "Count/mL")
new_class_MQ(my_data)
```

---

on\_plate\_selection      *Sort experimental design on graphical 96-well-plate*

---

**Description**

Loads user's data, prompt a graphical representation of a 96 well plate and let the user select where the duplicates of each condition were placed. Use for reordering excel file. Plate image with selection can also be saved in the form of a png file in the "specified\_path/output\_MQ" directory.

**Usage**

```
on_plate_selection(MACSQuant, number_of_replicates, number_of_conditions,
  control=FALSE, save.files=FALSE)
```

**Arguments**

MACSQuant	object of class MACSQuant resulting of the function load_maxQuant(). Contains the original data table
number_of_replicates	For each condition, the number of duplicates (must be the same for all conditions)
number_of_conditions	The number of conditions tested (eg: Drug 1 alone, Drug 2 alone)
control	Is there a control in this experiment (eg: Staurosporin)
save.files	Used to save the image in the output folder

**Value**

A formatted report file along with intermediates results

**Examples**

```
print("run manually, requires user input")
# on_plate_selection(MACSQuant,3,5)
# let you select 5 conditions of 3 replicates each
```

---

pipeline	<i>pipeline with report generation</i>
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---

**Description**

Loads user's data, prompt a graphical representation of a 96 well plate and let the user select where the duplicates of each condition were placed. Use for reordering excel file. Plate image with selection can also be saved in the form of a png file in the output\_MQ directory.

Also generates a complete report with the graphics

**Usage**

```
pipeline(filepath, sheet_name=NULL, number_of_replicates, number_of_conditions,
control=FALSE, save.files=TRUE, MACSQuant.obj=NULL)
```

**Arguments**

filepath	path of the excel file
sheet_name	Name of the sheet to load (optional, first sheet is default)
number_of_replicates	For each condition, the number of duplicates (must be the same for all conditions)
number_of_conditions	The number of conditions tested (eg: Drug 1 alone, Drug 2 alone)
control	Is there a control in this experiment (eg: Staurosporin)
save.files	Used to save the image in the output folder
MACSQuant.obj	object of class MACSQuant

**Value**

A formatted report file along with intermediates results

**Examples**

```
print("run manually, requires user input")
filepath <- system.file("extdata", "SingleDrugs.xlsx",
  package = "MACSQuantifyR")
# pipeline(filepath,3,5)
# let you select 5 conditions of 3 replicates each
```



---

rData	<i>accessor function to access raw data</i>
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---

**Description**

This function allows the user to access raw data table

**Usage**

```
rData(MACSQuant)
```

**Arguments**

MACSQuant	object of class MACSQuant resulting of the function load_maxQuant(). Contains the original data table
-----------	---

**Value**

the raw data table

**Examples**

```
filepath <- system.file("extdata", "SingleDrugs.xlsx",  
  package = "MACSQuantifyR")  
#MACSQuant = load_MACSQuant(filepath)  
  
#rData(MACSQuant)
```

---

setPath	<i>sets custom output path</i>
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---

**Description**

This function allows the user to set the output directory path

**Usage**

```
setPath(MACSQuant, path=NULL)
```

**Arguments**

MACSQuant	object of class MACSQuant resulting of the function load_maxQuant(). Contains the original data table
path	user defined path, default is tempd

**Value**

object of class MACSQuant with updated path

**Examples**

```
filepath <- system.file("extdata", "SingleDrugs.xlsx",
  package = "MACSQuantifyR")
#MACSQuant = load_MACSQuant(filepath)
user_path="."
#MACSQuant = setPath(MACSQuant,path=user_path)
```

---

sorted

*accessor function to access sorted data*

---

**Description**

This function allows the user to access sorted data table

**Usage**

```
sorted(MACSQuant)
```

**Arguments**

MACSQuant      object of class MACSQuant resulting of the function load\_maxQuant(). Contains the original data table

**Value**

the raw data table

**Examples**

```
filepath <- system.file("extdata", "SingleDrugs.xlsx",
  package = "MACSQuantifyR")
#MACSQuant = load_MACSQuant(filepath)

#sorted(MACSQuant)
```

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