# Package 'PvSTATEM'

July 21, 2025

Description Speeds up the process of loading raw data from MBA (Multiplex Bead Assay) examina-

**Title** Reading, Quality Control and Preprocessing of MBA (Multiplex

Type Package

Bead Assay) Data

```
tions, performs quality control checks, and automatically normalises the data, prepar-
      ing it for more advanced, downstream tasks. The main objective of the package is to create a sim-
      ple environment for a user, who does not necessarily have experience with R lan-
      guage. The package is developed within the project of the same name - 'PvS-
      TATEM', which is an international project aiming for malaria elimination.
BugReports https://github.com/mini-pw/PvSTATEM/issues
Version 0.2.2
License BSD_3_clause + file LICENSE
Encoding UTF-8
RoxygenNote 7.3.2
Imports dplyr, ggplot2, nplr, R6, readr, readxl, stringi, stringr,
      grid, png, tools, ggrepel, lubridate, R.utils, syglite, fs,
      scales
Suggests knitr, qpdf, rmarkdown, testthat (>= 3.0.0)
Config/testfhat/edition 3
VignetteBuilder knitr
URL https://github.com/mini-pw/PvSTATEM,
      https://mini-pw.github.io/PvSTATEM/
NeedsCompilation no
Author Tymoteusz Kwiecinski [aut, cre] (ORCID:
       <https://orcid.org/0009-0006-7362-9821>),
      Jakub Grzywaczewski [aut],
      Mateusz Nizwantowski [aut],
      Przemyslaw Biecek [ths] (ORCID:
       <a href="https://orcid.org/0000-0001-8423-1823">https://orcid.org/0000-0001-8423-1823>),</a>
      Nuno Sepulveda [ths] (ORCID: <a href="https://orcid.org/0000-0002-8542-1706">https://orcid.org/0000-0002-8542-1706</a>)
```

Maintainer Tymoteusz Kwiecinski <tymoteuszkwiecinski@gmail.com>

Repository CRAN

**Date/Publication** 2025-02-27 00:30:02 UTC

# **Contents**

create_standard_curve_model_analyte	2
generate_levey_jennings_report	3
generate_plate_report	5
get_nmfi	6
handle_high_dose_hook	8
is_valid_data_type	9
is_valid_sample_type	9
Model	10
Plate	13
PlateBuilder	18
plot_counts	21
plot_layout	22
plot_levey_jennings	23
plot_mfi_for_analyte	24
plot_standard_curve_analyte	25
plot_standard_curve_analyte_with_model	26
plot_standard_curve_stacked	27
predict.Model	29
process_dir	29
process_file	31
process_plate	32
read_intelliflex_format	34
read_layout_data	35
read_luminex_data	35
read_xponent_format	37
translate_sample_names_to_sample_types	38
	40
	generate_levey_jennings_report generate_plate_report get_nmfi handle_high_dose_hook is_valid_data_type is_valid_sample_type  Model Plate PlateBuilder plot_counts plot_layout plot_levey_jennings plot_mfi_for_analyte plot_standard_curve_analyte_vlot_standard_curve_analyte_vlot_standard_curve_stacked predict.Model process_dir process_file process_plate read_intelliflex_format read_layout_data read_luminex_data read_xponent_format

 ${\tt create\_standard\_curve\_model\_analyte}$ 

Create a standard curve model for a certain analyte

## Description

Create a standard curve model for a certain analyte

## Usage

```
create_standard_curve_model_analyte(
  plate,
  analyte_name,
  data_type = "Median",
  source_mfi_range_from_all_analytes = FALSE,
  detect_high_dose_hook = TRUE,
  ...
)
```

## **Arguments**

(Plate()) Object of the Plate class plate analyte\_name (character(1)) Name of the analyte for which we want to create the model data\_type (character(1)) Data type of the value we want to use to fit the model - the same datatype as in the plate file. By default, it equals to Median source\_mfi\_range\_from\_all\_analytes (logical(1)) If TRUE, the MFI range is calculated from all analytes; if FALSE, the MFI range is calculated only for the current analyte Defaults to FALSE detect\_high\_dose\_hook (logical(1)) If TRUE, the high dose hook effect is detected and handled. For more information, please see the handle\_high\_dose\_hook function documentation. Additional arguments passed to the model Standard curve samples should not contain na values in mfi values nor in dilu-

#### Value

(Model()) Standard Curve model

tions.

```
generate_levey_jennings_report
```

Generate a Levey-Jennings Report for Multiple Plates.

## Description

This function generates a Levey-Jennings report for a list of plates. The report includes layout plot, levey jennings plot, for each analyte and selected dilutions. The report also includes stacked standard curves plot in both monochromatic and color versions for each analyte. The report is generated using the levey\_jennings\_report\_template.Rmd template.

#### Usage

```
generate_levey_jennings_report(
  list_of_plates,
  report_title,
  dilutions = c("1/100", "1/400"),
  filename = NULL,
  output_dir = "reports",
  additional_notes = NULL
)
```

#### **Arguments**

 $list\_of\_plates$  A list of plate objects.

report\_title (character(1)) The title of the report.

dilutions (character) A character vector specifying the dilutions to be included in the

report. Default is c("1/100", "1/400").

filename (character(1)) The name of the output HTML report file. If not provided

or set to NULL, the filename will be based on the first plate name, formatted as {plate\_name}\_levey\_jennings.html. If the filename does not contain the .html extension, it will be automatically added. Absolute file paths in filename will override output\_dir. Existing files at the specified path will be overwrit-

ten.

output\_dir (character(1)) The directory where the report will be saved. Defaults to 're-

ports'. If NULL, the current working directory will be used. Necessary directories

will be created if they do not exist.

additional\_notes

(character(1)) Additional notes to be included in the report. Markdown formatting is supported. If not provided, the section will be omitted.

#### Value

A Levey-Jennings report in HTML format.

## **Examples**

```
output_dir <- tempdir(check = TRUE)

dir_with_luminex_files <- system.file("extdata", "multiplate_lite",
    package = "PvSTATEM", mustWork = TRUE
)
list_of_plates <- process_dir(dir_with_luminex_files,
    return_plates = TRUE, format = "xPONENT", output_dir = output_dir
)
note <- "This is a Levey-Jennings report.\n**Author**: Jane Doe \n**Tester**: John Doe"

generate_levey_jennings_report(
    list_of_plates = list_of_plates,
    report_title = "QC Report",</pre>
```

generate\_plate\_report 5

```
dilutions = c("1/100", "1/200"),
  output_dir = tempdir(),
  additional_notes = note
)
```

generate\_plate\_report Generate a report for a plate.

#### **Description**

This function generates a report for a plate. The report contains all the necessary information about the plate, from the general plate parameters, such as examination date, to the breakdown of the analytes' plots. The report is generated using the plate\_report\_template.Rmd template.

## Usage

```
generate_plate_report(
  plate,
  use_model = TRUE,
  filename = NULL,
  output_dir = "reports",
  counts_lower_threshold = 50,
  counts_higher_threshold = 70,
  additional_notes = NULL
)
```

#### **Arguments**

plate A plate object.

use\_model (logical(1)) A logical value indicating whether the model should be used in

the report.

filename (character(1)) The name of the output HTML report file. If not provided or

equals to NULL, the output filename will be based on the plate name, precisely: {plate\_name}\_report.html. By default the plate\_name is the filename of the input file that contains the plate data. For more details please refer to Plate.

If the passed filename does not contain .html extension, the default extension .html will be added. Filename can also be a path to a file, e.g. path/to/file.html. In this case, the output\_dir and filename will be joined together. However, if the passed filepath is an absolute path and the output\_dir parameter is also provided, the output\_dir parameter will be ignored. If a file already exists under a greatified filepath the function will everywrite it.

under a specified filepath, the function will overwrite it.

output\_dir (character(1)) The directory where the output CSV file should be saved. Please note that any directory path provided will create all necessary directories (in-

cluding parent directories) if they do not exist. If it equals to NULL the current

working directory will be used. Default is 'reports'.

6 get\_nmfi

#### Value

A report.

#### **Examples**

```
plate_file <- system.file("extdata", "CovidOISExPONTENT_CO_reduced.csv", package = "PvSTATEM")
# a plate file with reduced number of analytes to speed up the computation
layout_file <- system.file("extdata", "CovidOISExPONTENT_CO_layout.xlsx", package = "PvSTATEM")
note <- "This is a test report.\n**Author**: Jane Doe \n**Tester**: John Doe"

plate <- read_luminex_data(plate_file, layout_file, verbose = FALSE)
example_dir <- tempdir(check = TRUE) # a temporary directory
generate_plate_report(plate,
   output_dir = example_dir,
   counts_lower_threshold = 40,
   counts_higher_threshold = 50,
   additional_notes = note
)</pre>
```

get\_nmfi

Calculate normalised MFI values for a plate

#### Description

The function calculates the normalised MFI (nMFI) values for each of the analytes in the plate.

The nMFI values are calculated as the ratio of the test samples' MFI values to the standard curve samples with the target dilution.

When nMFI could be used? In general, it is preferred to use Relative Antibody Unit (RAU) values for any analysis. However, it is sometimes impossible to fit a model to the standard curve samples. This may happen if the MFI values of test samples are much higher than the MFI of standard curve samples. Then, the prediction would require significant data extrapolation, which could lead to unreliable results.

In such cases, the nMFI values could be used as a proxy for RAU values if we want, for instance, to account for plate-to-plate variation.

get\_nmfi 7

#### Usage

```
get_nmfi(
  plate,
  reference_dilution = 1/400,
  data_type = "Median",
  verbose = TRUE
)
```

#### **Arguments**

plate (Plate()) a plate object for which to calculate the nMFI values

reference\_dilution

(numeric(1) or character(1)) the dilution value of the standard curve sample to use as a reference for normalisation. The default is 1/400. It should refer to a dilution of a standard curve sample in the given plate object. This parameter could be either a numeric value or a string. In case it is a character string, it should have format 1/d+, where d+ is any positive integer.

data\_type

(character(1)) type of data for the computation. Median is the default

# Value

verbose

nmfi (data.frame) a data frame with normalised MFI values for each analyte in the plate and all test samples.

(logical(1)) print additional information. The default is TRUE

## **Examples**

```
# read the plate
plate_file <- system.file("extdata", "CovidOISExPONTENT.csv", package = "PvSTATEM")
layout_file <- system.file("extdata", "CovidOISExPONTENT_layout.csv", package = "PvSTATEM")

plate <- read_luminex_data(plate_file, layout_file)

# artificially bump up the MFI values of the test samples (the Median data type is default one)
plate$data[["Median"]][plate$sample_types == "TEST", ] <-
    plate$data[["Median"]][plate$sample_types == "TEST", ] * 10

# calculate the nMFI values
nmfi <- get_nmfi(plate, reference_dilution = 1 / 400)

# we don't do any extrapolation and the values should be comparable across plates
head(nmfi)
# different params
nmfi <- get_nmfi(plate, reference_dilution = "1/50")</pre>
```

#### **Description**

Typically, the MFI values associated with standard curve samples should decrease as we dilute the samples. However, sometimes in high dilutions, the MFI presents a non monotonic behavior. In that case, MFI values associated with dilutions above (or equal to) high\_dose\_threshold should be removed from the analysis.

For more information about this effect please refer to: Namburi, R. P. et. al. (2014) High-dose hook effect.

For the nplr model the recommended number of standard curve samples is at least 4. If the high dose hook effect is detected but the number of samples below the high\_dose\_threshold is lower than 4, additional warning is printed and the samples are not removed.

The function returns a logical vector that can be used to subset the MFI values.

#### Usage

```
handle_high_dose_hook(mfi, dilutions, high_dose_threshold = 1/200)
```

## **Arguments**

```
mfi (numeric())
dilutions (numeric())
high_dose_threshold
```

(numeric(1)) MFI values associated with dilutions above this threshold should be checked for the high dose hook effect

#### Value

```
sample selector (logical())
```

## **Examples**

```
plate_filepath <- system.file(
    "extdata", "CovidOISExPONTENT.csv",
    package = "PvSTATEM", mustWork = TRUE
) # get the filepath of the csv dataset
layout_filepath <- system.file(
    "extdata", "CovidOISExPONTENT_layout.xlsx",
    package = "PvSTATEM", mustWork = TRUE
)
plate <- read_luminex_data(plate_filepath, layout_filepath) # read the data
# here we plot the data with observed high dose hook effect
plot_standard_curve_analyte(plate, "RBD_omicron")</pre>
```

is\_valid\_data\_type 9

```
# here we create the model with the high dose hook effect handled
model <- create_standard_curve_model_analyte(plate, "RBD_omicron")</pre>
```

is\_valid\_data\_type

Check validity of given data type

## Description

Check if the data type is valid. The data type is valid if it is one of the elements of the VALID\_DATA\_TYPES vector. The valid data types are:

```
c(Median, Net MFI, Count, Avg Net MFI, Mean, Peak).
```

## Usage

```
is_valid_data_type(data_type)
```

#### **Arguments**

data\_type

A string representing the data type.

## Value

TRUE if the data type is valid, FALSE otherwise.

```
is_valid_sample_type Check validity of given sample type
```

## Description

Check if the sample type is valid. The sample type is valid if it is one of the elements of the VALID\_SAMPLE\_TYPES vector. The valid sample types are:

```
c(ALL, BLANK, TEST, NEGATIVE CONTROL, STANDARD CURVE, POSITIVE CONTROL).
```

## Usage

```
is_valid_sample_type(sample_type)
```

## **Arguments**

sample\_type

A string representing the sample type.

#### Value

TRUE if the sample type is valid, FALSE otherwise.

10 Model

Model

Logistic regression model for the standard curve

## **Description**

The Model class is a wrapper around the nplr model. It allows to predict the RAU (Relative Antibody Unit) values directly from the MFI values of a given sample.

The nplr model is fitted using the formula:

$$y = B + \frac{T - B}{(1 + 10^{b \cdot (x_{mid} - x)})^s},$$

where:

- y is the predicted value, MFI in our case,
- x is the independent variable, dilution in our case,
- $\bullet$  B is the bottom plateau the right horizontal asymptote,
- T is the top plateau the left horizontal asymptote,
- b is the slope of the curve at the inflection point,
- $x_{mid}$  is the x-coordinate at the inflection point,
- s is the asymmetric coefficient.

This equation is referred to as the Richards' equation. More information about the model can be found in the nplr package documentation.

After the model is fitted to the data, the RAU values can be predicted using the predict method. The RAU value is simply a predicted dilution value (using the standard curve) for a given MFI multiplied by 1,000 000 to have a more readable value. For more information about the differences between dilution, RAU and MFI values, please see the "Normalisation" section in the "Basic PvSTATEM functionalities" vignette.

#### **Public fields**

```
analyte (character(1))
Name of the analyte for which the model was fitted

dilutions (numeric())
Dilutions used to fit the model

mfi (numeric())
MFI values used to fit the model

mfi_min (numeric(1))
Minimum MFI used for scaling MFI values to the range [0, 1]

mfi_max (numeric(1))
Maximum MFI used for scaling MFI values to the range [0, 1]

model (nplr)
Instance of the nplr model fitted to the data
```

Model 11

```
log_dilution (logical())
         Indicator should the dilutions be transformed using the log10 function
    log_mfi (logical())
         Indicator should the MFI values be transformed using the log10 function
    scale_mfi (logical())
         Indicator should the MFI values be scaled to the range [0, 1]
Active bindings
    top_asymptote (numeric(1))
         The top asymptote of the logistic curve
    bottom_asymptote (numeric(1))
         The bottom asymptote of the logistic curve
Methods
     Public methods:
        • Model$new()
        • Model$predict()
        • Model$get_plot_data()
        • Model$print()
        • Model$clone()
     Method new(): Create a new instance of Model R6 class
       Usage:
       Model$new(
         analyte,
         dilutions,
         mfi,
         npars = 5,
         verbose = TRUE,
         log_dilution = TRUE,
         log_mfi = TRUE,
         scale_mfi = TRUE,
         mfi_min = NULL,
         mfi_max = NULL
       Arguments:
       analyte (character(1))
           Name of the analyte for which the model was fitted.
       dilutions (numeric())
           Dilutions used to fit the model
       mfi MFI(numeric())
           values used to fit the model
       npars (numeric(1))
           Number of parameters to use in the model
```

12 Model

```
verbose (logical())
     If TRUE prints messages, TRUE by default
 log_dilution (logical())
     If TRUE the dilutions are transformed using the log10 function, TRUE by default
 log_mfi (logical())
     If TRUE the MFI values are transformed using the log10 function, TRUE by default
 scale_mfi (logical())
     If TRUE the MFI values are scaled to the range [0, 1], TRUE by default
 mfi_min (numeric(1))
     Enables to set the minimum MFI value used for scaling MFI values to the range [0, 1]. Use
     values before any transformations (e.g., before the log10 transformation)
 mfi_max (numeric(1))
     Enables to set the maximum MFI value used for scaling MFI values to the range [0, 1]. Use
     values before any transformations (e.g., before the log10 transformation)
Method predict(): Predict RAU values from the MFI values
 Usage:
 Model$predict(mfi, over_max_extrapolation = 0, eps = 1e-06)
 Arguments:
 mfi (numeric())
     MFI values for which we want to predict the RAU values
 over_max_extrapolation (numeric(1))
     How much we can extrapolate the values above the maximum RAU value seen in stan-
     dard curve samples RAU_{max}. Defaults to 0. If the value of the predicted RAU is above
     RAU_{max} + over_max_extrapolation, the value is censored to the value of that sum.
 eps (numeric(1))
     A small value used to avoid numerical issues close to the asymptotes
 Returns: (data.frame())
 Dataframe with the predicted RAU values for given MFI values The columns are named as
 follows:
   • RAU - the Relative Antibody Units (RAU) value
   • MFI - the predicted MFI value
Method get_plot_data(): Data that can be used to plot the standard curve.
 Usage:
 Model$get_plot_data()
 Returns: (data.frame())
 Prediction dataframe for scaled MFI (or logMFI) values in the range [0, 1]. Columns are named
 as in the predict method
Method print(): Function prints the basic information about the model such as the number of
parameters or samples used
 Usage:
 Model$print()
```

**Method** clone(): The objects of this class are cloneable with this method.

```
Usage:
Model$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

## **Examples**

```
plate_file <- system.file("extdata", "CovidOISExPONTENT.csv", package = "PvSTATEM")
layout_file <- system.file("extdata", "CovidOISExPONTENT_layout.csv", package = "PvSTATEM")
plate <- read_luminex_data(plate_file, layout_filepath = layout_file)
model <- create_standard_curve_model_analyte(plate, "S2", log_mfi = TRUE)
print(model)</pre>
```

Plate

Plate object

## **Description**

A class to represent the luminex plate. It contains information about the samples and analytes that were examined on the plate as well as some additional metadata and batch info

## **Public fields**

```
plate_name (character(1))
```

Name of the plate. Set to the name of the file from which the plate was read.

```
analyte_names (character())
```

Names of the analytes that were examined on the plate.

```
sample_names (character())
```

Names of the samples that were examined on the plate. The order of the samples in this vector is identical with order in the CSV source file.

```
batch_name (character(1))
```

Name of the batch to which the plate belongs.

```
plate_datetime (POSIXct())
```

A date and time when the plate was created by the machine

```
sample_locations (character())
```

Locations of the samples on the plate. This vector is in the same order as the sample\_names vector.

```
sample_types (character())
```

Types of the samples that were examined on the plate. The possible values are c(ALL, BLANK, TEST, NEGATIVE CONTROL, STANDARD CURVE, POSITIVE CONTROL). This vector is in the same order as the sample\_names vector.

```
dilutions (character())
```

A list containing names of the samples as keys and string representing dilutions as values. The dilutions are represented as strings. This vector is in the same order as the sample\_names vector.

```
dilution_values (numeric())
```

A list containing names of the samples as keys and numeric values representing dilutions as values. It is in the same order as the sample\_names vector.

```
default_data_type (character(1))
```

The default data type that will be returned by the get\_data method. By default is set to Median.

```
data (list())
```

A list containing dataframes with the data for each sample and analyte. The possible data types - the keys of the list are:

```
c(Median, Net MFI, Count, Avg Net MFI, Mean, Peak).
```

In each dataframe, the rows represent samples and the columns represent analytes.

```
batch_info (list())
```

A list containing additional, technical information about the batch.

```
layout (character())
```

A list containing information about the layout of the plate. The layout is read from the separate file and usually provides additional information about the dilutions, sample names, and the sample layout on the actual plate.

```
blank_adjusted (logical)
```

A flag indicating whether the blank values have been adjusted.

#### Methods

## **Public methods:**

- Plate\$new()
- Plate\$print()
- Plate\$summary()
- Plate\$get\_data()
- Plate\$get\_dilution()
- Plate\$get\_dilution\_values()
- Plate\$blank\_adjustment()
- Plate\$clone()

#### **Method** new(): Method to initialize the Plate object

```
Usage:
Plate$new(
   plate_name,
   sample_names,
   analyte_names,
   batch_name = "",
   plate_datetime = NULL,
   sample_locations = NULL,
```

```
sample_types = NULL,
  dilutions = NULL,
  dilution_values = NULL,
  default_data_type = NULL,
  data = NULL,
  batch_info = NULL,
  layout = NULL
Arguments:
plate_name (character(1))
    Name of the plate. By default is set to an empty string, during the reading process it is set
    to the name of the file from which the plate was read.
sample_names (character())
    Names of the samples that were examined on the plate.
analyte_names (character())
    Names of the analytes that were examined on the plate.
batch_name (character(1))
    Name of the batch to which the plate belongs. By default is set to an empty string, during
    the reading process it is set to the batch field of the plate
plate_datetime (POSIXct())
    Datetime object representing the date and time when the plate was created by the machine.
sample_locations (character())
    Locations of the samples on the plate.
sample_types (character())
    Types of the samples that were examined on the plate. The possible values are
    c(ALL, BLANK, TEST, NEGATIVE CONTROL, STANDARD CURVE, POSITIVE CONTROL).
dilutions (character())
    A list containing names of the samples as keys and string representing dilutions as values.
    The dilutions are represented as strings.
dilution_values (numeric())
    A list containing names of the samples as keys and numeric values representing dilutions as
    values.
default_data_type (character(1))
    The default data type that will be returned by the get_data method. By default is set to
    Median.
data (list())
    A list containing dataframes with the data for each sample and analyte. The possible data
    types - the keys of the list are
    c (Median, Net MFI, Count, Avg Net MFI, Mean, Peak). In each dataframe, the rows rep-
    resent samples and the columns represent analytes.
batch_info (list())
    A list containing additional, technical information about the batch.
layout (character())
```

A list containing information about the layout of the plate. The layout is read from the separate file and usually provides additional information about the dilutions, sample names, and the sample layout on the actual plate.

**Method** print(): Function prints the basic information about the plate such as the number of samples and analytes

```
Usage:
Plate$print(...)
Arguments:
```

... Additional parameters to be passed to the print function Print the summary of the plate

**Method** summary(): Function outputs basic information about the plate, such as examination date, batch name, and sample types.

Usage:

```
Plate$summary(..., include_names = FALSE)
```

Arguments:

... Additional parameters to be passed to the print function Get data for a specific analyte and sample type

include\_names If include\_names parameter is TRUE, a part from count of control samples, provides also their names. By default FALSE

**Method** get\_data(): Function returns data for a specific analyte and sample.

```
Usage:
```

```
Plate$get_data(
   analyte,
   sample_type = "ALL",
   data_type = self$default_data_type
)
```

Arguments:

analyte An analyte name or its id of which data we want to extract. If set to 'ALL' returns data for all analytes.

sample\_type is a type of the sample we want to extract data from. The possible values are c(ALL, BLANK, TEST, NEGATIVE CONTROL, STANDARD CURVE, POSITIVE CONTROL). Default value is ALL.

data\_type The parameter specifying which data type should be returned. This parameter has to take one of values:

c(Median, Net MFI, Count, Avg Net MFI, Mean, Peak). What's more, the data\_type has to be present in the plate's data Default value is plate's default\_data\_type, which is usually Median.

*Returns:* Dataframe containing information about a given sample type and analyte Get the string representation of dilutions

**Method** get\_dilution(): Function returns the dilution represented as strings for a specific sample type.

```
Usage:
```

```
Plate$get_dilution(sample_type)
```

Arguments:

sample\_type type of the samples that we want to obtain the dilution for. The possible values are

c(ALL, BLANK, TEST, NEGATIVE CONTROL, STANDARD CURVE, POSITIVE CONTROL) Default value is ALL.

*Returns:* A list containing names of the samples as keys and string representing dilutions as values. Get the numeric representation of dilutions

**Method** get\_dilution\_values(): Function returns the dilution values for a specific sample type.

Usage:

Plate\$get\_dilution\_values(sample\_type)

Arguments:

sample\_type type of the samples that we want to obtain the dilution values for. The possible values are

c(ALL, BLANK, TEST, NEGATIVE CONTROL, STANDARD CURVE, POSITIVE CONTROL) Default value is ALL.

*Returns:* A list containing names of the samples as keys and numeric values representing dilutions as values.

Adjust the MFI values by subtracting the background

**Method** blank\_adjustment(): Function adjusts the values of samples (all samples excluding the blanks) by clamping the values to the aggregated value of the BLANK samples for each analyte separately.

The purpose of this operation is to unify the data by clamping values below the background noise. how this method works was inspired by the paper https://doi.org/10.1038/s41598-020-57876-0 which covers the quality control in the MBA.

In short, this operation firstly calculates the aggregate of MFI in the BLANK samples (available methods are: min, max, mean, median) and then replaces all values below this threshold with the threshold value.

Method does not modifies the data of type Count.

This operation is recommended to be performed before any further analysis, but is optional. Skipping it before further analysis is allowed, but will result in a warning.

Usage:

```
Plate$blank_adjustment(threshold = "max", in_place = TRUE)
```

Arguments:

threshold The method used to calculate the background value for each analyte. Every value below this threshold will be clamped to the threshold value. By default max. Available methods are: min, max, mean, median.

in\_place Whether the method should produce new plate with adjusted values or not, By default TRUE - operates on the current plate.

**Method** clone(): The objects of this class are cloneable with this method.

Usage:

```
Plate$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

18 PlateBuilder

PlateBuilder

PlateBuilder

## **Description**

This class helps creating the Plate object. It is used to store the data and validate the final fields.

#### **Active bindings**

layout\_as\_vector Print the layout associated with the plate as a flattened vector of values.

#### Methods

#### **Public methods:**

- PlateBuilder\$new()
- PlateBuilder\$set\_sample\_locations()
- PlateBuilder\$set\_dilutions()
- PlateBuilder\$set\_sample\_types()
- PlateBuilder\$set\_sample\_names()
- PlateBuilder\$set\_plate\_datetime()
- PlateBuilder\$set\_data()
- PlateBuilder\$set\_default\_data\_type()
- PlateBuilder\$set\_batch\_info()
- PlateBuilder\$set\_plate\_name()
- PlateBuilder\$set\_layout()
- PlateBuilder\$build()
- PlateBuilder\$clone()

## Method new(): Initialize the PlateBuilder object

Usage:

PlateBuilder\$new(sample\_names, analyte\_names, batch\_name = "", verbose = TRUE)

Arguments:

sample\_names • vector of sample names measured during an examination in the same order as in the data

analyte\_names • vector of analytes names measured during an examination in the same order as in the data

batch\_name • name of the batch during which the plate was examined obtained from the plate info. An optional parameter, by default set to "" - an empty string.

verbose • logical value indicating whether to print additional information. This parameter is stored as a private attribute of the object and reused in other methods

**Method** set\_sample\_locations(): Set the sample types used during the examination *Usage*:

```
PlateBuilder$set_sample_locations(sample_locations)

Arguments:
sample_locations vector of sample locations pretty name ie. A1, B2
```

**Method** set\_dilutions(): Extract and set the dilutions from layout, sample names or use a provided vector of values. The provided vector should be the same length as the number of samples and should contain dilution factors saved as strings

Usage:

PlateBuilder\$set\_dilutions(use\_layout\_dilutions = TRUE, values = NULL)

Arguments.

use\_layout\_dilutions logical value indicating whether to use names extracted from layout files to extract dilutions. If set to FALSE the function uses the sample names as a source for dilution

values a vector of dilutions to overwrite the extraction process Set and extract sample types from the sample names. Optionally use the layout file to extract the sample types

Method set\_sample\_types():

Usage:

PlateBuilder\$set\_sample\_types(use\_layout\_types = TRUE, values = NULL)

Arguments:

use\_layout\_types logical value indicating whether to use names extracted from layout files to extract sample types

values a vector of sample types to overwrite the extraction process

**Method** set\_sample\_names(): Set the sample names used during the examination. If the layout is provided, extract the sample names from the layout file. Otherwise, uses the original sample names from the Luminex file

Usage:

PlateBuilder\$set\_sample\_names(use\_layout\_sample\_names = TRUE)

Arguments:

use\_layout\_sample\_names logical value indicating whether to use names extracted from layout files. If set to false, this function only checks if the sample names are provided in the plate

**Method** set\_plate\_datetime(): Set the plate datetime for the plate

Usage.

PlateBuilder\$set\_plate\_datetime(plate\_datetime)

Arguments:

plate\_datetime a POSIXct datetime object representing the date and time of the examination

Method set\_data(): Set the data used during the examination

Usage:

PlateBuilder\$set\_data(data)

20 PlateBuilder

#### Arguments:

data a named list of data frames containing information about the samples and analytes. The list is named by the type of the data e.g. Median, Net MFI, etc. The data frames contain information about the samples and analytes The rows are different measures, whereas the columns represent different analytes Example of how data\$Median looks like:

Sample	Analyte1	Analyte2	Analyte3
Sample1	1.2	2.3	3.4
Sample2	4.5	5.6	6.7
Sample96	7.8	8.9	9.0

**Method** set\_default\_data\_type(): Set the data type used for calculations

Usage:

PlateBuilder\$set\_default\_data\_type(data\_type = "Median")

Arguments:

data\_type a character value representing the type of data that is currently used for calculations. By default, it is set to Median

Method set\_batch\_info(): Set the batch info for the plate

Usage.

PlateBuilder\$set\_batch\_info(batch\_info)

Arguments:

batch\_info a raw list containing metadata about the plate read from the Luminex file

**Method** set\_plate\_name(): Set the plate name for the plate. The plate name is extracted from the filepath

Usage:

PlateBuilder\$set\_plate\_name(file\_path)

Arguments:

file\_path a character value representing the path to the file

**Method** set\_layout(): Set the layout matrix for the plate. This function performs basic validation

• verifies if the plate is a matrix of shape 8x12 with 96 wells

Usage:

PlateBuilder\$set\_layout(layout\_matrix)

Arguments:

layout\_matrix a matrix containing information about the sample names. dilutions, etc.

Method build(): Create a Plate object from the PlateBuilder object

Usage:

PlateBuilder\$build(validate = TRUE)

plot\_counts 21

```
Method clone(): The objects of this class are cloneable with this method.
    Usage:
    PlateBuilder$clone(deep = FALSE)
    Arguments:
    deep Whether to make a deep clone.
```

plot\_counts

Plot counts in a 96-well plate

## Description

This function plots counts in a 96-well plate using a colour to represent the count ranges. There is a possibility of plotting exact counts in each well.

If the plot window is resized, it's best to re-run the function to adjust the scaling. Sometimes, when a legend is plotted, the whole layout may be shifted. It's best to stretch the window, and everything will be adjusted automatically.

## Usage

```
plot_counts(
   plate,
   analyte_name,
   plot_counts = TRUE,
   plot_legend = FALSE,
   lower_threshold = 50,
   higher_threshold = 70
)
```

## **Arguments**

plate The plate object with the counts data

plot\_counts Logical indicating if the counts should be plotted plot\_legend Logical indicating if the legend should be plotted

lower\_threshold

The lower threshold for the counts, it separates green and yellow colours

higher\_threshold

The higher threshold for the counts, it separates yellow and red colours

## Value

A ggplot object

22 plot\_layout

## **Examples**

```
plate_filepath <- system.file("extdata", "CovidOISExPONTENT_CO.csv",
    package = "PvSTATEM", mustWork = TRUE
)
layout_filepath <- system.file("extdata", "CovidOISExPONTENT_CO_layout.xlsx",
    package = "PvSTATEM", mustWork = TRUE
)
plate <- read_luminex_data(plate_filepath, layout_filepath)
plot_counts(
    plate = plate, analyte_name = "OC43_NP_NA",
    plot_counts = TRUE, plot_legend = FALSE
)</pre>
```

plot\_layout

Plot layout of a 96-well plate

## Description

This function plots the layout of a 96-well plate using a colour to represent the sample types.

If the plot window is resized, it's best to re-run the function to adjust the scaling. Sometimes, the whole layout may be shifted when a legend is plotted. It's best to stretch the window, and everything will be adjusted automatically.

#### Usage

```
plot_layout(plate, plot_legend = TRUE)
```

## Arguments

plate The plate object with the layout information plot\_legend Logical indicating if the legend should be plotted

#### Value

A ggplot object

#### **Examples**

```
plate_filepath <- system.file("extdata", "CovidOISExPONTENT_CO.csv",
    package = "PvSTATEM", mustWork = TRUE
)
layout_filepath <- system.file("extdata", "CovidOISExPONTENT_CO_layout.xlsx",
    package = "PvSTATEM", mustWork = TRUE
)
plate <- read_luminex_data(plate_filepath, layout_filepath)
plot_layout(plate = plate, plot_legend = TRUE)</pre>
```

plot\_levey\_jennings 23

## **Description**

The function plots a Levey-Jennings chart for the given analyte in the list of plates. The Levey-Jennings chart is a graphical representation of the data that enables the detection of outliers and trends. It is a quality control tool that is widely used in the laboratories across the world.

## Usage

```
plot_levey_jennings(
    list_of_plates,
    analyte_name,
    dilution = "1/400",
    sd_lines = c(1.96),
    data_type = "Median"
)
```

## Arguments

```
list_of_plates A list of plate objects for which to plot the Levey-Jennings chart

analyte_name (character(1)) the analyte for which to plot the Levey-Jennings chart

dilution (character(1)) the dilution for which to plot the Levey-Jennings chart. The
    default is "1/400"

sd_lines (numeric) the vector of coefficients for the standard deviation lines to plot, for
    example, c(1.96, 2.58) will plot four horizontal lines: mean +/- 1.96sd, mean
    +/- 2.58sd default is c(1.96) which will plot two lines mean +/- 1.96*sd

data_type (character(1)) the type of data used plot. The default is "Median"
```

#### Value

A ggplot object with the Levey-Jennings chart

## **Examples**

```
# creating temporary directory for the example
output_dir <- tempdir(check = TRUE)

dir_with_luminex_files <- system.file("extdata", "multiplate_reallife_reduced",
    package = "PvSTATEM", mustWork = TRUE
)
list_of_plates <- process_dir(dir_with_luminex_files,
    return_plates = TRUE, format = "xPONENT", output_dir = output_dir
)
list_of_plates <- rep(list_of_plates, 10) # since we have only 3 plates i will repeat them 10 times</pre>
```

24 plot\_mfi\_for\_analyte

```
plot\_levey\_jennings(list\_of\_plates, "ME", dilution = "1/400", sd\_lines = c(0.5, 1, 1.96, 2.58))
```

```
{\tt plot\_mfi\_for\_analyte} \quad \textit{Plot MFI value distribution for a given analyte}
```

## Description

Plot MFI value distribution for a given analyte

## Usage

```
plot_mfi_for_analyte(
   plate,
   analyte_name,
   data_type = "Median",
   plot_type = "violin",
   scale_y = "log10",
   plot_outliers = FALSE
)
```

## Arguments

plate	A plate object
analyte_name	The analyte to plot
data_type	The type of data to plot. Default is "Median"
plot_type	The type of plot to generate. Default is "violin". Available options are "boxplot" and "violin".
scale_y	What kind of transformation of the scale to apply. By default MFI is presented in a "log10" scale. Available options are described in the documentation of scale_y_continuous undertransform parameter.
plot_outliers	When using "boxplot" type of a plot one can set this parameter to TRUE and display the names of samples for which MFI falls outside the 1.5 IQR interval

#### Value

A ggplot object

```
plot_standard_curve_analyte

Standard curves
```

## **Description**

Plot standard curve samples of a plate of a given analyte.

## Usage

```
plot_standard_curve_analyte(
   plate,
   analyte_name,
   data_type = "Median",
   decreasing_rau_order = TRUE,
   log_scale = c("all"),
   plot_line = TRUE,
   plot_blank_mean = TRUE,
   plot_rau_bounds = TRUE,
   plot_legend = TRUE,
   verbose = TRUE
)
```

## Arguments

plate A plate object analyte\_name Name of the analyte of which standard curve we want to plot. data\_type Data type of the value we want to plot - the same datatype as in the plate file. By default equals to Net MFI decreasing\_rau\_order If TRUE the RAU values are plotted in decreasing order, TRUE by default Which elements on the plot should be displayed in log scale. By default "RAU". log\_scale If NULL or c() no log scale is used, if "all" or c("RAU", "MFI") all elements are displayed in log scale. If TRUE a line is plotted, TRUE by default plot\_line plot\_blank\_mean If TRUE the mean of the blank samples is plotted, TRUE by default plot\_rau\_bounds If TRUE the RAU values bounds are plotted, TRUE by default plot\_legend If TRUE the legend is plotted, TRUE by default If TRUE prints messages, TRUE by default verbose

## Value

ggplot object with the plot

## **Examples**

```
path <- system.file("extdata", "CovidOISExPONTENT.csv",
    package = "PvSTATEM", mustWork = TRUE
)
layout_path <- system.file("extdata", "CovidOISExPONTENT_layout.xlsx",
    package = "PvSTATEM", mustWork = TRUE
)
plate <- read_luminex_data(path, layout_filepath = layout_path, verbose = FALSE)
plot_standard_curve_analyte(plate, "Spike_6P", plot_legend = FALSE, data_type = "Median")</pre>
```

plot\_standard\_curve\_analyte\_with\_model

Plot standard curve of a certain analyte with fitted model

## Description

Function plots the values of standard curve samples and the fitted model.

## Usage

```
plot_standard_curve_analyte_with_model(
   plate,
   model,
   data_type = "Median",
   decreasing_rau_order = TRUE,
   log_scale = c("all"),
   plot_asymptote = TRUE,
   plot_test_predictions = TRUE,
   plot_blank_mean = TRUE,
   plot_rau_bounds = TRUE,
   plot_legend = TRUE,
   verbose = TRUE,
   ...
)
```

#### **Arguments**

plate Plate object

model fitted Model object, which predictions we want to plot

data\_type Data type of the value we want to plot - the same datatype as in the plate file.

By default equals to Median

decreasing\_rau\_order

If TRUE the RAU values are plotted in decreasing order, TRUE by default.

log\_scale Which elements on the plot should be displayed in log scale. By default "all".

If NULL or c() no log scale is used, if "all" or c("RAU", "MFI") all elements

are displayed in log scale.

```
plot_asymptote If TRUE the asymptotes are plotted, TRUE by default

plot_test_predictions

If TRUE the predictions for the test samples are plotted, TRUE by default. The

predictions are obtained through extrapolation of the model

plot_blank_mean

If TRUE the mean of the blank samples is plotted, TRUE by default

plot_rau_bounds

If TRUE the RAU bounds are plotted, TRUE by default

plot_legend

If TRUE the legend is plotted, TRUE by default

verbose

If TRUE prints messages, TRUE by default

Additional arguments passed to the predict function
```

#### Value

a ggplot object with the plot

#### **Examples**

```
path <- system.file("extdata", "CovidOISExPONTENT.csv",
    package = "PvSTATEM", mustWork = TRUE
)
layout_path <- system.file("extdata", "CovidOISExPONTENT_layout.xlsx",
    package = "PvSTATEM", mustWork = TRUE
)
plate <- read_luminex_data(path, layout_filepath = layout_path, verbose = FALSE)
model <- create_standard_curve_model_analyte(plate, analyte_name = "Spike_B16172")
plot_standard_curve_analyte_with_model(plate, model, decreasing_rau_order = FALSE)</pre>
```

```
plot_standard_curve_stacked
```

Standard curve stacked plot for levey-jennings report

## Description

Function generates a plot of stacked on top of each other standard curves for a given analyte form a list of plates. The plot is created with the levey-jennings report in mind, but it can be run by itself.

## Usage

```
plot_standard_curve_stacked(
    list_of_plates,
    analyte_name,
    data_type = "Median",
    decreasing_dilution_order = TRUE,
    monochromatic = TRUE,
    legend_type = NULL,
```

```
log_scale = c("all"),
verbose = TRUE
)
```

#### **Arguments**

list\_of\_plates list of Plate objects

analyte\_name Name of the analyte of which standard curves we want to plot.

data\_type Data type of the value we want to plot - the same datatype as in the plate file.

By default equals to Median

decreasing\_dilution\_order

If TRUE the dilution values are plotted in decreasing order, TRUE by default

monochromatic If TRUE the color of standard curves changes from white (the oldest) to blue (the

newest) it helps to observe drift in calibration of the device; otherwise, more

varied colours are used, TRUE by default

legend\_type default value is NULL, then legend type is determined based on monochromatic

value. If monochromatic is equal to TRUE then legend type is set to date, if it is FALSE then legend type is set to plate\_name. User can override this behavior

by setting explicitly legend\_type to date or plate\_name.

log\_scale Which elements on the plot should be displayed in log scale. By default "all".

If NULL or c() no log scale is used, if "all" or c("dilutions", "MFI") all

elements are displayed in log scale.

verbose If TRUE prints messages, TRUE by default

## Value

ggplot object with the plot

#### **Examples**

```
# creating temporary directory for the example
output_dir <- tempdir(check = TRUE)

dir_with_luminex_files <- system.file("extdata", "multiplate_reallife_reduced",
    package = "PvSTATEM", mustWork = TRUE
)
list_of_plates <- process_dir(dir_with_luminex_files,
    return_plates = TRUE, format = "xPONENT", output_dir = output_dir
)
plot_standard_curve_stacked(list_of_plates, "ME", data_type = "Median", monochromatic = FALSE)</pre>
```

predict.Model 29

predict.Model

Predict the RAU values from the MFI values

## **Description**

More details can be found here: Model

## Usage

```
## S3 method for class 'Model'
predict(object, mfi, ...)
```

## **Arguments**

object (Model()) Object of the Model class

mfi (numeric()) MFI values for which we want to predict the RAU values Should

be in the same scale as the MFI values used to fit the model

... Additional arguments passed to the method

#### Value

```
(data.frame())
```

process\_dir

Process a dir of files to generate normalised data and reports

## **Description**

The output files will be created alongside their corresponding input files, preserving the directory structure of the input directory unless the flatten\_output\_dir parameter is set to TRUE.

# Usage

```
process_dir(
  input_dir,
  output_dir = NULL,
  recurse = FALSE,
  flatten_output_dir = FALSE,
  layout_filepath = NULL,
  format = NULL,
  normalisation_types = c("RAU", "nMFI"),
  generate_reports = FALSE,
  merge_outputs = FALSE,
  column_collision_strategy = "intersection",
  return_plates = FALSE,
```

30 process\_dir

```
dry_run = FALSE,
  verbose = TRUE,
   ...
)
```

#### **Arguments**

input\_dir (character(1)) The directory containing the input files. It may be nested.

output\_dir (character(1)) Optional overwrite directory where the output files should be

saved. The default is NULL. By default, the output directory is the same as the

input directory.

recurse (logical(1)) If TRUE, the function will search for files recursively in the input

directory. The default is FALSE.

flatten\_output\_dir

(logical(1)) If TRUE, the output files will be saved in the output directory di-

rectly. The default is FALSE.

layout\_filepath

 $({\tt character(1)})\ The\ path\ to\ the\ layout\ file.\ The\ default\ is\ {\tt NULL},\ and\ the\ layout$ 

file will have to be determined automatically based on the file name.

format (character(1)) The format of the Luminex data. The default is NULL, and

the format will have to be determined automatically based on the file name. Available options are xPONENT and INTELLIFLEX.

normalisation\_types

(character()) A vector of normalisation types to use. The default is c("RAU",

"nMFI").

generate\_reports

(logical(1)) If TRUE, generate quality control reports for each file. The default

is FALSE.

merge\_outputs (logical(1)) If TRUE, merge the outputs of all plates into a single CSV file for

each normalisation type. The resulting file will be saved in the output directory with the name merged\_{normalisation\_type}\_{timestamp}.csv. Example:

merged\_nMFI\_20250115\_230735.csv.

column\_collision\_strategy

(character(1)) A method for handling missing or additional columns when merging outputs. Possible options are union and intersection. The default is

intersection.

return\_plates (logical(1)) If TRUE, return a list of processed plates. The default is FALSE.

dry\_run (logical(1)) If TRUE, the function will not process any files but will print the

information about the files that would be processed. The default is FALSE.

verbose (logical(1)) Print additional information. The default is TRUE.

... Additional arguments to for the process\_file function.

## Value

If the return\_plates parameter is set to TRUE the function returns a list of plates sorted by the plate\_datetime (The time of the experiment noted in the csv file) in increasing order (oldest plates first). If the return\_plates parameters is set to FALSE the function returns NULL.

process\_file 31

## **Examples**

```
# Select input directory to process
dir <- system.file("extdata", "multiplate_lite", package = "PvSTATEM", mustWork = TRUE)
# Select output directory
output_dir <- tempdir(check = TRUE)
# Process input directory and return plates
plates <- process_dir(dir, return_plates = TRUE, output_dir = output_dir)</pre>
```

process\_file

Process a file to generate normalised data and reports

## **Description**

Perform process\_plate and generate\_plate\_report for a given plate file. In more detail, this function reads the plate file and calls the process\_plate on the processed plate objects across all the normalisation types, including the raw MFI values. If the user has specified the generate\_report flag, it will also call the generate\_plate\_report function generating the quality control report.

#### Usage

```
process_file(
  plate_filepath,
  layout_filepath,
  output_dir = "normalised_data",
  format = "xPONENT",
  generate_report = FALSE,
  process_plate = TRUE,
  normalisation_types = c("RAU", "nMFI"),
  verbose = TRUE,
  ...
)
```

## **Arguments**

32 process\_plate

## **Examples**

```
# Select an input csv file for processing and corresponding layout file
plate_file <- system.file("extdata", "CovidOISExPONTENT_CO_reduced.csv", package = "PvSTATEM")
layout_file <- system.file("extdata", "CovidOISExPONTENT_CO_layout.xlsx", package = "PvSTATEM")

example_dir <- tempdir(check = TRUE) # a temporary directory
# create and save dataframe with computed dilutions for all suported noramlization types
process_file(plate_file, layout_file, output_dir = example_dir)

example_dir2 <- tempdir(check = TRUE) # a temporary directory
# process the plate for a specific normalization type
process_file(plate_file, layout_file, output_dir = example_dir2, normalisation_types = c("RAU"))</pre>
```

process\_plate

Process a plate and save output values to a CSV

## **Description**

Depending on the normalisation\_type argument, the function will compute the RAU or nMFI values for each analyte in the plate. RAU is the default normalisation type.

The behaviour of the function, in the case of RAU normalisation type, can be summarised as follows:

- 1. Adjust blanks if not already done.
- 2. Fit a model to each analyte using standard curve samples.
- 3. Compute RAU values for each analyte using the corresponding model.
- 4. Aggregate computed RAU values into a single data frame.
- 5. Save the computed RAU values to a CSV file.

More info about the RAU normalisation can be found in  $create\_standard\_curve\_model\_analyte$  function documentation  $create\_standard\_curve\_model\_analyte$  or in the Model reference Model.

In case the normalisation type is **nMFI**, the function will:

- 1. Adjust blanks if not already done.
- 2. Compute nMFI values for each analyte using the target dilution.
- 3. Aggregate computed nMFI values into a single data frame.
- 4. Save the computed nMFI values to a CSV file.

More info about the nMFI normalisation can be found in get\_nmfi function documentation get\_nmfi.

process\_plate 33

## Usage

```
process_plate(
  plate,
  filename = NULL,
  output_dir = "normalised_data",
  write_output = TRUE,
  normalisation_type = "RAU",
  data_type = "Median",
  include_raw_mfi = TRUE,
  adjust_blanks = FALSE,
  verbose = TRUE,
  reference_dilution = 1/400,
  ...
)
```

#### **Arguments**

plate

(Plate()) a plate object

filename

(character(1)) The name of the output CSV file with normalised MFI values. If not provided or equals to NULL, the output filename will be based on the normalisation type and the plate name, precisely: {plate\_name}\_{normalisation\_type}.csv. By default the plate\_name is the filename of the input file that contains the plate data. For more details please refer to Plate.

If the passed filename does not contain .csv extension, the default extension .csv will be added. Filename can also be a path to a file, e.g. path/to/file.csv. In this case, the output\_dir and filename will be joined together. However, if the passed filepath is an absolute path and the output\_dir parameter is also provided, the output\_dir parameter will be ignored. If a file already exists under a specified filepath, the function will overwrite it.

output\_dir

(character(1)) The directory where the output CSV file should be saved. Please note that any directory path provided will create all necessary directories (including parent directories) if they do not exist. If it equals to NULL the current working directory will be used. Default is 'normalised\_data'.

write\_output

(logical(1)) whether or not to write the output to a file specified by filename parameter. The default is TRUE.

normalisation\_type

(character(1)) type of normalisation to use. Available options are: c(RAU, nMFI).

c(R

 $({\tt character(1)}) \ type \ of \ data \ to \ use \ for \ the \ computation. \ Median \ is \ the \ default$ 

include\_raw\_mfi

data\_type

(logical(1)) include raw MFI values in the output. The default is TRUE. In case this option is TRUE, the output dataframe contains two columns for each analyte: one for the normalised values and one for the raw MFI values. The normalised columns are named as AnalyteName and AnalyteName\_raw, respectively.

adjust\_blanks

(logical(1)) adjust blanks before computing RAU values. The default is FALSE

verbose

(logical(1)) print additional information. The default is TRUE

reference\_dilution

(numeric(1)) target dilution to use as reference for the nMFI normalisation. Ignored in case of RAU normalisation. Default is 1/400. It should refer to a dilution of a standard curve sample in the given plate object. This parameter could be either a numeric value or a string. In case it is a character string, it should have the format 1/d+, where d+ is any positive integer.

Additional arguments to be passed to the fit model function (create\_standard\_curve\_model\_analyte)

#### Value

. . .

a data frame with normalised values

#### **Examples**

```
plate_file <- system.file("extdata", "CovidOISExPONTENT_CO_reduced.csv", package = "PvSTATEM")</pre>
# a plate file with reduced number of analytes to speed up the computation
layout_file <- system.file("extdata", "CovidOISExPONTENT_CO_layout.xlsx", package = "PvSTATEM")</pre>
plate <- read_luminex_data(plate_file, layout_file, verbose = FALSE)</pre>
example_dir <- tempdir(check = TRUE) # a temporary directory</pre>
# create and save dataframe with computed dilutions
process_plate(plate, output_dir = example_dir)
# process plate without adjusting blanks and save the output to a file with a custom name
process_plate(plate,
  filename = "plate_without_blanks_adjusted.csv",
  output_dir = example_dir, adjust_blanks = FALSE
)
# nMFI normalisation
process_plate(plate,
  output_dir = example_dir,
  normalisation_type = "nMFI", reference_dilution = 1 / 400
)
```

read\_intelliflex\_format

Read the Intelliflex format data

#### **Description**

Read the Intelliflex format data

## Usage

```
read_intelliflex_format(path, verbose = TRUE)
```

read\_layout\_data 35

## **Arguments**

path Path to the INTELLIFLEX file

verbose Print additional information. Default is TRUE

read\_layout\_data

Read layout data from a file

## **Description**

Read layout data from a file

#### Usage

```
read_layout_data(layout_file_path, ...)
```

#### **Arguments**

layout\_file\_path

Path to the layout file

... Additional arguments to pass to the underlying read function

## Value

A matrix with the layout data. The row names are supposed to be letters A,B,C, etc. The column names are supposed to be numbers 1,2,3, etc.

read\_luminex\_data

Read Luminex Data

## **Description**

Reads a file containing Luminex data and returns a Plate object. If provided, can also read a layout file, which usually contains information about the sample names, sample types or its dilutions.

The function is capable of reading data in two different formats:

- xPONENT
- INTELLIFLEX which are produced by two different Luminex machines.

36 read\_luminex\_data

#### Usage

```
read_luminex_data(
  plate_filepath,
  layout_filepath = NULL,
  format = "xPONENT",
  plate_file_separator = ",",
  plate_file_encoding = "UTF-8",
  use_layout_sample_names = TRUE,
  use_layout_types = TRUE,
  use_layout_dilutions = TRUE,
  default_data_type = "Median",
  sample_types = NULL,
  dilutions = NULL,
  verbose = TRUE
)
```

## **Arguments**

```
plate_filepath Path to the Luminex plate file

layout_filepath Path to the Luminex layout file

format The format of the Luminex data. Select from: xPONENT, INTELLIFLEX plate_file_separator

The separator used in the plate file
```

plate\_file\_encoding

The encoding used in the plate file

use\_layout\_sample\_names

Whether to use names from the layout file in extracting sample names.

use\_layout\_types

Whether to use names from the layout file in extracting sample types. Works only when layout file is provided

use\_layout\_dilutions

Whether to use dilutions from the layout file in extracting dilutions. Works only when layout file is provided

default\_data\_type

The default data type to use if none is specified

sample\_types a vector of sample types to use instead of the extracted ones dilutions a vector of dilutions to use instead of the extracted ones

verbose Whether to print additional information and warnings. TRUE by default

#### Value

Plate file containing the Luminex data

read\_xponent\_format 37

#### **Examples**

```
plate_file <- system.file("extdata", "CovidOISExPONTENT.csv", package = "PvSTATEM")
layout_file <- system.file("extdata", "CovidOISExPONTENT_layout.csv", package = "PvSTATEM")
plate <- read_luminex_data(plate_file, layout_file)

plate_file <- system.file("extdata", "CovidOISExPONTENT_CO.csv", package = "PvSTATEM")
layout_file <- system.file("extdata", "CovidOISExPONTENT_CO_layout.xlsx", package = "PvSTATEM")
# To suppress warnings and additional information use verbose = FALSE
plate <- read_luminex_data(plate_file, layout_file, verbose = FALSE)</pre>
```

read\_xponent\_format

Read the xPONENT format data

## **Description**

Read the xPONENT format data

## Usage

```
read_xponent_format(
  path,
  exact_parse = FALSE,
  encoding = "utf-8",
  separator = ",",
  verbose = TRUE
)
```

#### **Arguments**

path Path to the xPONENT file

exact\_parse Whether to parse the file exactly or not Exact parsing means that the batch,

calibration and assay metadata will be parsed as well

encoding Encoding of the file

separator Separator for the CSV values

verbose Whether to print the progress. Default is TRUE

## **Description**

Function translates sample names to sample types based on the sample name from Luminex file and the sample name from the layout file, which may not be provided. The function uses regular expressions to match the sample names to the sample types.

It parses the names as follows:

If  $sample\_names$  or  $sample\_names\_from\_layout$  equals to BLANK, BACKGROUND or B, then SampleType equals to BLANK

If sample\_names or sample\_names\_from\_layout equals to STANDARD CURVE, SC, S, contains substring 1/d+ and has prefix , S\_, S or CP3, then SampleType equals to STANDARD CURVE

If sample\_names or sample\_names\_from\_layout equals to NEGATIVE CONTROL, N, or contains substring NEG, then SampleType equals to NEGATIVE CONTROL

If sample\_names or sample\_names\_from\_layout starts with P followed by whitespace, POS followed by whitespace, some sample name followed by substring 1/\d+ SampleType equals to POSITIVE CONTROL

Otherwise, the returned SampleType is TEST

## Usage

```
translate_sample_names_to_sample_types(
  sample_names,
  sample_names_from_layout = NULL
)
```

## Arguments

Vector of sample names from Layout file values in this vector may be different than sample\_names and may contain additional information about the sample type like dilution. This vector when set has to have at least the length of sample\_names.

#### Value

A vector of valid sample\_type strings of length equal to the length of sample\_names

# Examples

```
translate\_sample\_names\_to\_sample\_types(c("B", "BLANK", "NEG", "TEST1")) \\ translate\_sample\_names\_to\_sample\_types(c("S", "CP3")) \\
```

# **Index**

```
create_standard_curve_model_analyte, 2,
generate_levey_jennings_report, 3
generate_plate_report, 5
get_nmfi, 6, 32
handle_high_dose_hook, 3, 8
is_valid_data_type, 9
is_valid_sample_type, 9
Model, 10, 29, 32
Plate, 5, 13, 33
PlateBuilder, 18
plot_counts, 21
plot_layout, 22
plot_levey_jennings, 23
plot_mfi_for_analyte, 24
plot_standard_curve_analyte, 25
plot_standard_curve_analyte_with_model,
        26
plot_standard_curve_stacked, 27
predict.Model, 29
process_dir, 29
process_file, 31
process_plate, 32
read_intelliflex_format, 34
read_layout_data, 35
read_luminex_data, 35
read_xponent_format, 37
scale_y_continuous, 24
translate_sample_names_to_sample_types,
```