

Package ‘PKbioanalysis’

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Type Package

Title Pharmacokinetic Bioanalysis Experiments Design and Exploration

Version 0.3.0

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Description Automate pharmacokinetic/pharmacodynamic bioanalytical procedures based on best practices and regulatory recommendations.

The package impose regulatory constrains and sanity checking for common bioanalytical procedures.

Additionally, 'PKbioanalysis' provides a relational infrastructure for plate management and injection sequence.

License AGPL (>= 3)

Encoding UTF-8

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Depends R (>= 4.3.0)

Imports dplyr (>= 1.1.3), tidyselect, stringr (>= 1.5.1), ggplot2 (>= 3.5.1), ggforce (>= 0.4.1), tidyr (>= 1.3.0), glue (>= 1.6.2), checkmate, shiny (>= 1.9.1), DBI, duckdb (>= 1.0.0), bslib, bsicons, shinyWidgets, shinyjs, DiagrammeR, units, DT, stats, shinyalert, htmltools, rlang, grDevices, utils, yaml, rhandsontable, methods

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

URL <https://omarashkar.github.io/PKbioanalysis/>

BugReports <https://github.com/OmarAshkar/PKbioanalysis/issues>

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add_blank	<i>Add blank to the plate Can be either double blank (DB), CS0IS+ or CS1IS-</i>
-----------	---

Description

Add blank to the plate Can be either double blank (DB), CS0IS+ or CS1IS-

Usage

add_blank(plate, IS = TRUE, analyte = FALSE)

Arguments

- | | |
|---------|--|
| plate | PlateObj object |
| IS | logical. If TRUE, add IS to the well. |
| analyte | logical. If TRUE, add analyte to the well. |

Value

PlateObj

add_cs_curve	<i>Add calibration curve to the plate</i>
--------------	---

Description

Add calibration curve to the plate

Usage

```
add_cs_curve(plate, plate_std, rep = 1)
```

Arguments

plate	PlateObj
plate_std	character
rep	numeric. Number of replicates. Default is 1.

Value

PlateObj

Examples

```
plate <- generate_96() |>  
  add_cs_curve(c(1, 3, 5, 10, 50, 100, 200))  
plot(plate)
```

add_DB	<i>Add double blank (DB) to a plate</i>
--------	---

Description

Add double blank (DB) to a plate

Usage

```
add_DB(plate)
```

Arguments

plate	PlateObj object
-------	-----------------

Value

PlateObj

Examples

```
plate <- generate_96() |>
add_DB()
```

add_DQC	<i>Add dilution quality control (DQC) to the plate</i>
---------	--

Description

Add dilution quality control (DQC) to the plate

Usage

```
add_DQC(plate, conc, fac, rep = 5)
```

Arguments

plate	PlateObj object
conc	numeric. Concentration of the DQC well.
fac	numeric. Factor of the DQC well.
rep	numeric. Number of replicates. Default is 5. The current implementation does not check ULOQ or LLOQ boundaries.

add_QC	<i>Add quality control samples to the plate</i>
--------	---

Description

A function to add QCs to plate. This function assumes adherence to ICH guideline M10 on bioanalytical method validation and study sample analysis Geneva, Switzerland (2022). If you are not following this guideline, you can set 'reg = TRUE' to ignore the restrictions.

Usage

```
add_QC(
  plate,
  lqc_conc,
  mqc_conc,
  hqc_conc,
  extra = NULL,
  n_qc = 3,
  qc_serial = TRUE,
  reg = TRUE
)
```

Arguments

plate	PlateObj object
lqc_conc	low quality control concentration
mqc_conc	medium quality control concentration
hqc_conc	high quality control concentration
extra	numeric vector of extra QC concentrations. Default is NULL.
n_qc	number of QC sets. Default is 3
qc_serial	logical. If TRUE, QCs are placed serially
reg	logical. Indicates if restrictions should not be applied to the QC samples. Default is TRUE

Value

PlateObj

add_samples	<i>Add unknown samples to a plate</i>
-------------	---------------------------------------

Description

Add unknown samples to a plate

Usage

```
add_samples(
  plate,
  samples,
  time = NA,
  conc = NA,
  dil = NA,
  factor = NA,
  dosage = NA,
  prefix = "S",
  vtime = FALSE
)
```

Arguments

plate	PlateObj
samples	A vector representing samples names. Must be unique.
time	A vector representing time points. If vtime = FALSE, time will propagate to all samples.
conc	A vector representing concentration. Must be same length as samples.

dil	A vector representing dilution factor. Must be same length as samples.
factor	A vector representing factor. Must be same length as samples.
dosage	A vector representing dosage. Must be same length as samples.
prefix	A prefix to be added before samples names. Default is "S"
vtime	A logical. If TRUE, time is a vector of sample length as samples. Default is FALSE.

Details

final name will be of form. Prefix-SampleName-Time-Concentration-Factor samples must be a unique vector and did not exist in the plate before. Time is either a vector or a single value. If it is a vector, it will be repeated for each sample. Conc, dil, factor and dosage are either a vector or a single value. If it is a vector, it must be the corresponding length of samples.

Value

PlateObj

Examples

```
plate <- generate_96() |>
  add_samples(paste0("T", 1:12))
```

add_samples_c	<i>Cartesian product of sample factors to a plate</i>
---------------	---

Description

Cartesian product of sample factors to a plate

Usage

```
add_samples_c(
  plate,
  n_rep,
  time = NA,
  conc = NA,
  factor = NA,
  dosage = NA,
  prefix = "S"
)
```

Arguments

plate	PlateObj
n_rep	number of samples to be added
time	A vector representing time points
conc	A vector representing concentration
factor	A vector representing factor
dosage	A vector representing dosage
prefix	A prefix to be added before samples names. Default is "S"

Details

This function is a variation of 'add_samples()' where size of inputs does not matter. The function will automatically create a combination of all sample names with time, concentration and factor. final name will be of form. Prefix-SampleName-Time-Concentration-Factor

Value

PlateObj

add_suitability	<i>Add suitability sample to the plate</i>
-----------------	--

Description

Add suitability sample to the plate

Usage

```
add_suitability(plate, conc, label = "suitability")
```

Arguments

plate	PlateObj object.
conc	numeric. Concentration of the suitability well.
label	character. Label for the suitability well. Default is "suitability".

Value

PlateObj

build_injec_seq	<i>Create Injection Sequence</i>
-----------------	----------------------------------

Description

Create Injection Sequence

Usage

```
build_injec_seq(
    plate,
    method,
    repeat_std = 1,
    repeat_qc = 1,
    repeat_analyte = 1,
    blank_after_top_conc = TRUE,
    blank_at_end = TRUE,
    system_suitability = 0,
    blank_every_n = NULL,
    inject_vol,
    descr = "",
    prefix = Sys.Date(),
    suffix = "1",
    tray = 1,
    explore_mode = FALSE,
    conc_df = NULL
)
```

Arguments

plate	PlateObj object
method	choose method from database
repeat_std	number of re-injections for calibration standards. Default is 1.
repeat_qc	number of re-injections for QC wells. Default is 1
repeat_analyte	number of re-injections for unknown samples. Default is 1
blank_after_top_conc	If TRUE, adding blank after high concentrations of standards and QCS.
blank_at_end	If True, adding blank at the end of queue.
system_suitability	Number of re-injections for suitability vial.
blank_every_n	If no QCs, frequency of injecting blanks between analytes.
inject_vol	volume of injection in micro liters.
descr	Run description.
prefix	string at the beginning of the filename. Default is today's date.

suffix	string to be added to the end of the filename. Default is "1".
tray	Location in sample manager.
explore_mode	options either TRUE or FALSE. Default if FALSE.
conc_df	data.frame matching compound name to a scaling factor. Maximum 20 compounds allowed.

Details

explore_mode controls if exploratory samples are to be injected. A random sample from each CS and QC group will be sampled along with 1 blank sample.

Value

InjecListObj object

combine_injec_lists	<i>Create Sample List with rigorous design</i>
---------------------	--

Description

Create Sample List with rigorous design

Usage

```
combine_injec_lists(
  sample_lists,
  n_equi = 10,
  equi_pos,
  equi_prefix = Sys.Date(),
  equi_suffix = "equi",
  equi_injec_vol = 0.5
)
```

Arguments

sample_lists	a list of sample lists
n_equi	number of equilibration injections
equi_pos	position of equilibration injections. For format check details
equi_prefix	prefix for equilibration injections
equi_suffix	suffix for equilibration injections
equi_injec_vol	volume of equilibration injection

Details

The equi_pos format will be Row:Column format. E.g: "A,1"

Value

InjecListObj object

combine_plates	<i>Combine plates in MultiPlate object</i>
----------------	--

Description

Combine plates in MultiPlate object

Usage

combine_plates(plates)

Arguments

plates list of PlateObj objects

Value

MultiPlate object

download_sample_list	<i>Download sample list from database to local spreadsheet with vendor specific format</i>
----------------------	--

Description

Download sample list from database to local spreadsheet with vendor specific format

Usage

download_sample_list(sample_list, vendor)

Arguments

sample_list dataframe of sample list either from db or from write_injec_seq
vendor currently only 'masslynx', 'masshunter' and 'analyst' are supported

Details

For all current vendors, the exported format will be in csv format, compatible with the respective software.

Value

dataframe

fill_scheme	<i>Filling orientation of the plate</i>
-------------	---

Description

This function sets the filling scheme of the plate. The filling scheme is used to determine the order in which the samples are filled in the plate. The default filling scheme is horizontal, which means that the samples are filled from left to right and top to bottom. The vertical filling scheme means that the samples are filled from top to bottom and left to right.

Usage

```
fill_scheme(  
  plate,  
  fill = "h",  
  tbound = "A",  
  bbound = "H",  
  lbound = 1,  
  rbound = 12  
)
```

Arguments

plate	PlateObj
fill	character. Filling scheme. Either "h" for horizontal, "v" for vertical.
tbound	character. Top bound of the filling scheme. Default is "A"
bbound	character. Bottom bound of the filling scheme. Default is "H"
lbound	numeric. Left bound of the filling scheme. Default is 1
rbound	numeric. Right bound of the filling scheme. Default is 12

Value

PlateObj

generate_96	<i>Generate 96 Plate Generate a typical 96 well plate. User need to specify the empty rows which a going to be used across the experiment.</i>
-------------	--

Description

Generate 96 Plate Generate a typical 96 well plate. User need to specify the empty rows which a going to be used across the experiment.

Usage

```
generate_96(descr = "", start_row = "A", start_col = 1)
```

Arguments

descr	plate description.
start_row	A letter corresponding to empty rows in a 96 well plate. Default is A.
start_col	A number indicating a column number to start with, given the start row. Default is 1.

Value

PlateObj

Examples

```
plate <- generate_96()
plot(plate)

plate <- generate_96("calibration", start_row = "C", start_col = 11)
plot(plate)
```

length,MultiPlate-method

Length method for MultiPlate

Description

Length method for MultiPlate

Usage

```
## S4 method for signature 'MultiPlate'
length(x)
```

Arguments

x	MultiPlate object
---	-------------------

Value

number of plates

`make_calibration_study`*Create a calibration study with calibration standards and QCs*

Description

Create a calibration study with calibration standards and QCs

Usage

```
make_calibration_study(  
  plate,  
  plate_std,  
  lqc_conc = NULL,  
  mqc_conc = NULL,  
  hqc_conc = NULL,  
  n_qc = NULL,  
  qc_serial = FALSE,  
  n_CS0IS0 = 1,  
  n_CS0IS1 = 2,  
  n_CS1IS0 = 1  
)
```

Arguments

<code>plate</code>	PlateObj object
<code>plate_std</code>	vector of calibration standards
<code>lqc_conc</code>	LQC concentration
<code>mqc_conc</code>	MQC concentration
<code>hqc_conc</code>	HQC concentration
<code>n_qc</code>	number of QC sets
<code>qc_serial</code>	logical. If TRUE, QCs are placed serially
<code>n_CS0IS0</code>	number of CS0IS0 (double) blanks
<code>n_CS0IS1</code>	number of CS0IS1 blanks
<code>n_CS1IS0</code>	number of CS1IS0 blanks

Value

PlateObj

make_metabolic_study	Create a metabolic study layout
----------------------	---------------------------------

Description

Create a metabolic study layout

Usage

```
make_metabolic_study(  
  cmpds,  
  time_points = c(0, 5, 10, 15, 30, 45, 60, 75, 90, 120),  
  n_NAD = 3,  
  n_noNAD = 2  
)
```

Arguments

cmpds	vector of compounds, including any standards
time_points	vector of time points
n_NAD	number of NAD positive samples. Default is 3
n_noNAD	number of NAD negative samples. Default is 2

Details

Note that this function does not require plate object. It will create a plate object automatically and return MultiPlate object

Value

MultiPlate object

plate_app	bioanalytic_app
-----------	-----------------

Description

This function creates a shiny app for plate management

Usage

```
plate_app()
```

Value

A shiny app. No default return value. Can return a PlateObj if reuse_plate_button is clicked

plate_metadata	<i>Set plate description</i>
----------------	------------------------------

Description

Set plate description

Usage

plate_metadata(plate, descr)

Arguments

plate	PlateObj
descr	character. Description of the plate

Value

PlateObj

plot.PlateObj	<i>Plotting 96 well plate</i>
---------------	-------------------------------

Description

Plotting 96 well plate

Usage

```
## S3 method for class 'PlateObj'
plot(
  x,
  color = "conc",
  Instrument = "",
  caption = "",
  label_size = 1,
  transform_dil = FALSE,
  watermark = "auto",
  path = NULL,
  ...
)
```

Arguments

x	PlateObj
color	character. Coloring variable. Either "conc", "time", "factor", "samples", "dosage"
Instrument	A string placed at subtitle
caption	A string place at plate caption
label_size	numeric. Size of the label. Default is 15
transform_dil	logical. If TRUE, transform the dilution factor to the label
watermark	character. If "auto", a watermark is added to the plot. If "none", no watermark is added. Default is "auto"
path	Default is NULL, if not null, must be a path to save plate image
...	additional arguments passed to ggplot2::ggsave

Value

ggplot object

Examples

```
plate <- generate_96("new_plate", "C", 11) |>
  add_blank(IS = FALSE, analyte = FALSE) |>
  add_blank(IS = TRUE, analyte = FALSE) |>
  add_samples(c(
    "RD_per1", "RD_in1", "RD_T30", "RD_T60", "RD_T90", "RD_per2", "RD_in2",
    "EE_in0", "EE_T30", "EE_in30", "EE_T60", "EE_in60", "EE_T90", "EE_in90"
  ))
plot(plate)
```

plot_design

Plot the design of the plate

Description

Plot the design of the plate

Usage

```
plot_design(plate)
```

Arguments

plate	PlateObj object
-------	-----------------

Value

DiagrammeR object

register_plate	<i>Register a plate This will save the plate to the database</i>
----------------	--

Description

Register a plate This will save the plate to the database

Usage

register_plate(plate)

Arguments

plate PlateObj object or MultiPlate object

Value

PlateObj object or list of PlateObj objects

write_injec_seq	<i>Write injection sequence to database</i>
-----------------	---

Description

Write injection sequence to database

Usage

write_injec_seq(injec_seq)

Arguments

injec_seq InjecListObj object

Value

dataframe

[[,MultiPlate-method	<i>Subsetting method for MultiPlate</i>
----------------------	---

Description

Subsetting method for MultiPlate

Usage

```
## S4 method for signature 'MultiPlate'  
x[[i, j, ...]]
```

Arguments

x	MultiPlate object
i	index
j	index
...	additional arguments

Value

PlateObj object

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