

Package ‘PKbioanalysis’

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Type Package

Title Pharmacokinetic Bioanalysis Experiments Design and Exploration

Version 0.2.0

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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

RoxygenNote 7.3.2

Depends R (>= 4.1.0)

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

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

URL <https://github.com/OmarAshkar/PKbioanalysis>

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

Config/testthat/edition 3

VignetteBuilder knitr

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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)
```

Arguments

plate	PlateObj
plate_std	character

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_qcs *Add quality control samples to the plate*

Description

Add quality control samples to the plate

Usage

```
add_qcs(plate, lqc_conc, mqc_conc, hqc_conc, n_qc = 3, qc_serial = TRUE)
```

Arguments

plate	PlateObj object
lqc_conc	low quality control concentration
mqc_conc	medium quality control concentration
hqc_conc	high quality control concentration
n_qc	number of QC sets. Default is 3
qc_serial	logical. If TRUE, QCs are placed serially

Value

PlateObj

add_samples *Add unknown samples to a plate*

Description

Add unknown samples to a plate

Usage

```
add_samples(plate, samples, time = NA, conc = NA, factor = NA, prefix = "S")
```

Arguments

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

Details

final name will be of form. Prefix-SampleName-Time-Concentration-Factor

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, samples, time = NA, conc = NA, factor = NA, prefix = "S")
```

Arguments

plate	PlateObj
samples	A vector representing samples names
time	A vector representing time points
conc	A vector representing concentration
factor	A vector representing factor
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 *Add suitability sample to the plate*

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 *Create Injection Sequence*

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 *Create Sample List with rigorous design*

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</i>
----------------------	--

Description

Download sample list from database to local spreadsheet

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

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 = "", empty_rows = NULL, extra_fill = 0)
```

Arguments

descr	plate description.
empty_rows	vector of letters corresponding to empty rows in a 96 well plate.
extra_fill	additional spots to be ignored from the first empty row.

Value

PlateObj

Examples

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

plate <- generate_96("calibration", empty_rows = c("C", "D", "E"), extra_fill = 11)
plot(plate)
```

make_calibration_study	<i>Create a calibration study with calibration standards and QCs</i>
------------------------	--

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

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

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 = 15,
  path = NULL,
  ...
)
```

Arguments

x	PlateObj
color	character. Coloring variable. Either "conc", "time", "factor", "samples", "TYPE"
Instrument	A string placed at subtitle
caption	A string place at plate caption
label_size	numeric. Size of the label. Default is 15
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("C", "D", "E"), 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)
```

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>Export injection sequence to vendor specific format</i>
-----------------	--

Description

Export injection sequence to vendor specific format

Usage

```
write_injec_seq(injec_seq)
```

Arguments

injec_seq InjecListObj object

Value

dataframe

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