Package 'PKbioanalysis'

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Type Package

Title Pharmacokinetic Bioanalysis Experiments Design and Exploration

Version 0.5.0

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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 7.3.3

Depends R (>= 4.3.0)

Imports dplyr, tidyselect, stringr (>= 1.5.1), ggplot2, ggforce (>= 0.4.1), tidyr, glue (>= 1.6.2), checkmate, shiny, DBI, duckdb (>= 1.0.0), bslib, bsicons, cli, DiagrammeR, DT, shinyWidgets, shinyjs, units, stats, shinyalert, htmltools, rlang, grDevices, utils, yaml, rhandsontable, methods, reticulate (>= 1.44.1), RTMB, janitor, tibble, xml2, RaMS, data.tree, nloptr, forcats, ggiraph (>= 0.9.3), gt, plotly, pracma, reactable, gtools, ellmer, htmlwidgets, jsonlite, nlme, scales, shinychat, uuid, sortable, writexl

Suggests rxode2, knitr, patchwork, rmarkdown, testthat (>= 3.0.0)

SystemRequirements python (>= 3.10)

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

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

Config/testthat/edition 3

Collate 'PKbioanalysis-package.R' 'calc.R' 'chrom_anomaly_plots.R' 'chrom_app.R' 'chrom_parsers.R' 'chrom_utils.R' 'generics.R' 'class.R' 'chromatogram.R' 'config.R' 'dil_map.R'

'estim_residuals.R' 'genAI.R' 'gen_studydesign.R'
'generate_test_set.R' 'injec_list.R' 'linearitycheck.R'
'method_file.R' 'peak_integerate.R' 'plate.R' 'plate_expr.R'
'plates_class.R' 'process_chroms.R' 'quant_app.R'
'quant_misc.R' 'quant_object.R' 'quant_parsers.R'
'samples_profiles.R' 'study_app.R' 'suitability_utils.R'
'utils.R' 'writers.R' 'zzz.R'

NeedsCompilation no

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Contents

`add_blank` *Add blank to the plate Can be either double blank (DB), CS0IS+ or CS+IS0*

Description

Add blank to the plate Can be either double blank (DB), CS0IS+ or CS+IS0

Usage

```
add_blank(plate, IS = TRUE, analyte = FALSE, analytical = FALSE, group = NA)
```

Arguments

plate	PlateObj object
IS	logical. If TRUE, add IS to the well.
analyte	logical. If TRUE, add analyte to the well.
analytical	logical. If FALSE, the blank is analytical, if TRUE it is bioanalytical.
group	A string for bioanalytical group.

Value

PlateObj

---

add_cs_curve *Add calibration curve to the plate*

Description

Add calibration curve to the plate

Usage

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

Arguments

plate	PlateObj
plate_std	character
rep	numeric. Number of technical replicates. Default is 1.
group	A string for bioanalytical group.

Value

PlateObj

Examples

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

add_DB *Add double blank (DB) to a plate*

Description

Add double blank (DB) to a plate

Usage

```
add_DB(plate, analytical = FALSE, group = NA)
```

Arguments

plate	PlateObj object
analytical	logical. If TRUE, the blank is bioanalytical, if FALSE it is analytical.
group	A string for bioanalytical group.

Value

PlateObj

Examples

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

add_DQC *Add dilution quality control (DQC) to the plate*

Description

Add dilution quality control (DQC) to the plate

Usage

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

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.
group	A string for bioanalytical group. The current implementation does not check ULOQ or LLOQ boundaries.

add_QC *Add quality control samples to the plate*

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,
  group = NA
)
```

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.
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
group	A string for bioanalytical group.

Value

PlateObj

`add_samples` *Add samples to plate with pharmacokinetic attributes*

Description

Add samples to plate with pharmacokinetic attributes

Usage

```
add_samples(plate, samples, prefix = NA, dil = NA, group = NA, rep = 1)
```

Arguments

`plate`	PlateObj
`samples`	A vector representing samples names. Must be unique.
`prefix`	A prefix to be added before samples names. Default is "Sub".
`dil`	A vector representing samples' dilution factor. Must be same length as samples.
`group`	A vector representing samples' bioanalytical group. Must be same length as samples.
`rep`	Number of technical replicates for each combination. Default is 1.

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 dose are either a vector or a single value. If it is a vector, it must be the corrosponding length of samples.

Allowed routes are "IV", "IM", "IP", "SC", "PO", "INH" which are short for Intravenous, Intramuscular, Intraperitoneal, Subcutaneous, Per Os (oral), Inhalation.

Factor is an arbitrary factor used in the design like food vs fasted, healthy vs diseased, positive genotype ... etc.

Value

PlateObj

Examples

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

add_samples_db *Add samples from the sample log to the plate*

Description

Add samples from the sample log to the plate

Usage

```
add_samples_db(plate, logIds, dil = 1, namestyle = 1, group = NA)
```

Arguments

plate	PlateObj
logIds	A vector of log IDs from the sample log.
dil	A vector with length corresponding number of logIds. See details.
namestyle	A numeric value indicating the naming style. 1 for long names, 2 for short names.
group	A string for bioanalytical group.

Details

This function will retrieve sample information from the sample log database using the provided log IDs. It constructs sample names based on the specified naming style and adds them to the plate. The ‘dil‘ parameter allows specifying dilution factors for each sample, which will be appended to the sample names. If a single dilution factor is provided, it will be applied to all samples.

Value

PlateObj

add_samples_db2 *Add samples from the sample log to the plate with multiplication*

Description

Add samples from the sample log to the plate with multiplication

Usage

```
add_samples_db2(plate, logIds, dil = c(1, 1), namestyle = 1, group = NA)
```

Arguments

plate	PlateObj
logIds	A vector of log IDs from the sample log.
dil	A vector with length corresponding number of repeats. See details.
namestyle	A numeric value indicating the naming style. 1 for long names, 2 for short names.
group	A string for bioanalytical group.

Details

This function is wrapper around ‘add_samples_db()‘ that allows for quick replication of samples by dilution factor vector. For instance, it dil = c(1,10), the samples will repeated twice with one fold and 10 fold dilution factor each time.

---

add_suitability *Add suitability sample to the plate*

Description

Add suitability sample to the plate

Usage

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

Arguments

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

Value

PlateObj

area_report.PeakRes *gt table of areas*

Description

gt table of areas

Usage

```
area_report.PeakRes(
  peaks_res,
  normalize = TRUE,
  blanks = TRUE,
  analytes = TRUE,
  standards = TRUE,
  QCs = TRUE,
  compounds = NULL
)
```

Arguments

peaks_res	PeakRes object
normalize	logical. If TRUE, normalize the peak area by the IS area.
blanks	logical. If TRUE, include blanks
analytes	logical. If TRUE, include analytes
standards	logical. If TRUE, include standards
QCs	logical. If TRUE, include QCs
compounds	numeric vector of compound numbers to include. If NULL, include all compounds

calc_var_summary *Calculate Summary Statistics for Each Concentration Level For Either Concentration, Area, or Area Ratio*

Description

Calculate Summary Statistics for Each Concentration Level For Either Concentration, Area, or Area Ratio

Usage

```
calc_var_summary(
  df,
  col = "conc",
  acc_cutoff = 0.2,
  dev_cutoff = 0.2,
  type = "QC"
)
```

Arguments

df	Data frame with columns: stdconc (standardized concentration), conc (concentration), area (peak area), area_ratio (area ratio)
col	Column to calculate summary for ("conc", "area", or "area_ratio")
acc_cutoff	Accuracy threshold (default is 20%) for concentration vs standard concentration
dev_cutoff	Deviation threshold (default is 20%) for concentration vs standard concentration
type	Type of samples to include ("Standard", "QC", "DQC")

Author(s)

Omar I. Elashkar

---

check_chrom_cmpds *Check Matching of Compound and Transitions in chrom_res and method database*

Description

Check Matching of Compound and Transitions in chrom_res and method database

Usage

```
check_chrom_cmpds(chrom_res, method_id)
```

Arguments

chrom_res	ChromRes object
method_id	Method ID in the method database This is important to give no error before merging quantification results to ensure consistency.

Value

TRUE if all compounds and transitions match, otherwise FALSE

chrom_app *chrom_apps*

Description

This function creates a shiny app for peak integration.

Usage

```
chrom_app()
```

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 equilibriation injections
equi_pos	position of equilibriation injections. For format check details
equi_prefix	prefix for equilibriation injections
equi_suffix	suffix for equilibriation injections
equi_injec_vol	volume of equilibriation injection

Details

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

Value

InjecListObj object

combine_plates *Combine plates in MultiPlate object*

Description

Combine plates in MultiPlate object

Usage

```
combine_plates(plates)
```

Arguments

plates	list of PlateObj objects

Value

MultiPlate object

config_suitability *Configure suitability runs*

Description

Configure suitability runs by specifying vial position and range of runs to include.

Usage

```
config_suitability(quantres, vial_pos, start = NULL, end = NULL)
```

Arguments

quantres	QuantRes object
vial_pos	Vial position to use for suitability (e.g., "2:H,9")
start	Start position (1-based index) of runs to include. If NULL, starts from the first run.
end	End position (1-based index) of runs to include. If NULL, ends at the last run.

Value

Updated QuantRes object with suitability configuration.

create_new_study *Create a new study in the database*

Description

Create a new study in the database

Usage

```
create_new_study(df)
```

Arguments

df	A data frame with one row containing study details: type, title, description, pkstudy (logical), subject_type

Value

A data frame with the created study details including generated id, start_date, and status

cv *Calculate Coefficient of variation*

Description

Calculate Coefficient of variation

Usage

```
cv(x, percent = TRUE)
```

Arguments

x	vector
percent	To return the value as percentage

Details

A simple calculation of the coefficient of variation (CV) is done as the standard deviation divided by the mean. By default, the result is in percentage.

Value

numeric

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

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

`estim_dil_limit` *Estimate Dilution Limit Based on Additive and Proportional Errors and LLOQ*

Description

Estimate Dilution Limit Based on Additive and Proportional Errors and LLOQ

Usage

```
estim_dil_limit(add_err, prop_err, lloq)
```

Arguments

`add_err`	Additive error (constant)
`prop_err`	Proportional error (CV)
`lloq`	Lower limit of quantification

Author(s)

Omar I. Elashkar

Examples

```
estim_dil_limit(add_err=0.1, prop_err=0.1, lloq=1)
estim_dil_limit(add_err=1, prop_err=0.1, lloq=55)
```

---

estim_lloq *Estimate LLOQ From Existing Additive and Proportional errors*

Description

Estimate LLOQ From Existing Additive and Proportional errors

Usage

```
estim_lloq(add_err = 0.04, prop_err = 0.05, cv_lloq = 0.2, cv_lqc = 0.15)
```

Arguments

add_err	Additive error (constant)
prop_err	Proportional error (CV)
cv_lloq	Maximum coefficient of variation at LLOQ
cv_lqc	Maximum coefficient of variation at LQC
	A method to estimate LLOQ from existing additive and proportional errors. The function does inequality constrained optimization to find the LLOQ.

Author(s)

Omar I. Elashkar

---

export_integration *Export Expected RT*

Description

Export expected RT values for each peak in the chromatogram.

Usage

```
export_integration(chrom_res, path)
```

Arguments

chrom_res	ChromRes object
path	Path to save the file

`export_pk_profiles` *Export PK profiles for a given compound in a specified format Currently supports "nonmem" format. The exported file will include a CSV with the PK data and an Excel file with the codebook.*

Description

Export PK profiles for a given compound in a specified format Currently supports "nonmem" format. The exported file will include a CSV with the PK data and an Excel file with the codebook.

Usage

```
export_pk_profiles(x, compound_id, format = "NONMEM", filename = "data.zip")
```

Arguments

`x`	QuantRes object
`compound_id`	Compound ID for which to export PK profiles
`format`	Format to export (currently only "NONMEM" supported)
`filename`	Name of the output zip file (default: "data.zip")

Author(s)

Omar I. Elashkar

`export_run` *Export run*

Description

Export run

Usage

```
export_run(peaks_res, path)
```

Arguments

`peaks_res`	PeakRes object
`path`	path to save csv

extract_peak_bounds *Extract Peak Boundaries*

Description

Extract peak boundaries for all samples for a given compound ID

Usage

```
extract_peak_bounds(chrom_res, compound_id, samples_ids = NULL)
```

Arguments

chrom_res	ChromRes object
compound_id	Compound ID
samples_ids	Sample IDs. If NULL, all samples will be used The function automatically priortizes observed peak boundaries (manual integration) over expected ones. If observed boundaries are not available, it falls back to expected boundaries.

Value

Dataframe with compound_id, min, max

fill_scheme *Filling orientation of the plate*

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

---

filter_chrom *title Filter Chromatogram Peaks*

Description

This function filters chromatogram peaks based on transition ID and sample ID.

Usage

```
filter_chrom(
  chrom_res,
  transitions_ids = NULL,
  samples_id = NULL,
  cmpd_ids = NULL
)
```

Arguments

chrom_res	ChromRes object
transitions_ids	Vector of transition IDs to filter. If NULL, all transitions are returned.
samples_id	Sample ID to filter.
cmpd_ids	Compound ID to filter. It must be numeric. If NULL, all compounds are returned.

fit_var *Estimate Additive and proportional errors from calibration data*

Description

Estimate Additive and proportional errors from calibration data

Usage

```
fit_var(
  data,
  level = 0.95,
  method = "nlminb",
  bootstrap = FALSE,
  n_boot = 1000
)
```

Arguments

data	Data frame with columns: conc (concentration), stdconc (standardized concentration, e.g. conc/LLOQ)
level	Confidence level for the CI (default is 0.95)
method	Optimization method (default is "nlminb")
bootstrap	Logical indicating whether to perform bootstrap (default is TRUE)
n_boot	Number of bootstrap samples (default is 1000)

Author(s)

Omar I. Elashkar

formated_print *Format and print the results of fit_var*

Description

Format and print the results of fit_var

Usage

```
formated_print(x, digits = 3)
```

Arguments

x	Data frame with results
digits	Number of digits to display

Author(s)

Omar I. Elashkar

`generate_96` *Generate 96 well plate*

Description

Generate 96 well plate

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

Value

PlateObj

Examples

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

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

get_compound_ID *Find Compound ID from compound Name*

Description

This function returns the compound ID

Usage

```
get_compound_ID(chrom_res, compound_name)
```

Arguments

chrom_res	ChromRes object
compound_name	Compound Name

get_sample_ID *Find Sample ID from sample Name*

Description

This function returns the sample ID

Usage

```
get_sample_ID(chrom_res, sample_name)
```

Arguments

chrom_res	ChromRes object
sample_name	Sample Name

get_sample_names *Find sample names for all samples*

Description

Find sample names for all samples

Usage

```
get_sample_names(chrom_res)
```

Arguments

chrom_res	ChromRes object

Value

data.frame with sample and sample_id

has_default_bounds *check if default expected RT is set for a compound*

Description

check if default expected RT is set for a compound

Usage

```
has_default_bounds(chrom_res, compound_id)
```

Arguments

chrom_res	ChromRes object
compound_id	Compound ID

install_py_dep *Install Python dependencies for PKbioanalysis*

Description

Install Python dependencies for PKbioanalysis

Usage

```
install_py_dep(..., envname = "PKbioanalysis")
```

Arguments

...	Additional arguments passed to reticulate::py_install
envname	Name of the virtual environment to create/use. Default is "PKbioanalysis"

Value

None

integrate *integrate Peak with trapzoid method given start and end*

Description

integrate Peak with trapzoid method given start and end

Usage

```
integrate(chrom_res, compound_id, samples_ids, smoothed = TRUE)
```

Arguments

chrom_res	ChromRes object. Must have observed RT values
compound_id	Compound ID
samples_ids	Sample ID. If NULL, all samples will be used
smoothed	Logical. If TRUE, use smoothed chromatogram. Default is TRUE

is_integrated *Check if peak was integrated for a specific compound*

Description

Check if peak was integrated for a specific compound

Usage

```
is_integrated(chrom_res, compound_id, sample_id = NULL)

## S4 method for signature 'ChromRes'
is_integrated(chrom_res, compound_id, sample_id = NULL)

## S4 method for signature 'ChromResBase'
is_integrated(chrom_res, compound_id, sample_id = NULL)
```

Arguments

chrom_res	ChromRes or ChromResBase object
compound_id	Compound ID
sample_id	Sample ID. If NULL, all samples are checked

Value

logical

Examples

```
## Not run:
lapply(1:10, \(x) is_integrated(chrom_res, sample_id = 1, compound_id = 1))

## End(Not run)
```

is_smoothed *Return an indicator if the chromatogram is smoothed*

Description

Return an indicator if the chromatogram is smoothed

Usage

```
is_smoothed(chrom_res)
```

Arguments

chrom_res	ChromRes object

`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,
  group = NA
)
```

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
group	A string for bioanalytical group.

Value

PlateObj

---

make_metabolic_study *Create a metabolic study layout*

Description

Create a metabolic study layout

Usage

```
make_metabolic_study(
  study = "Metabolic Study",
  cmpds,
  time_points = c(0, 5, 10, 15, 30, 45, 60, 75, 90, 120),
  dose = NA,
  n_NAD = 3,
  n_noNAD = 2
)
```

Arguments

study	study name
cmpds	vector of compounds, including any standards
time_points	vector of time points
dose	dose amount. Default is NA
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

`nca_table` *Calculate Cmax, Tmax and AUC for each subject given a compound's PK profiles*

Description

Calculate Cmax, Tmax and AUC for each subject given a compound's PK profiles

Usage

```
nca_table(x, compound_id)
```

Arguments

`x`	QuantRes object with PK profiles extracted
`compound_id`	Compound ID for which to calculate NCA parameters

Details

This function calculates Cmax, Tmax and AUC for each subject given a compound's PK profiles.

Value

data frame with columns: subject_id, cmax, tmax, auc_last, compound_id

---

`pkmerge` *Merge PK profiles into QuantRes object*

Description

Merge PK profiles into QuantRes object

Usage

```
pkmerge(x)
```

Arguments

`x`	QuantRes object

plate_metadata *Set plate description*

Description

Set plate description

Usage

```
plate_metadata(plate, descr)
```

Arguments

plate	PlateObj
descr	character. Description of the plate

Value

PlateObj

plate_tree *Plot the design of the plate*

Description

Plot the design of the plate

Usage

```
plate_tree(plate, plot = TRUE)
```

Arguments

plate	PlateObj object
plot	logical. If TRUE, plot the tree

Value

data.tree Node object or DiagrammeR object plot_tree will focus only on bioanalytical vial types, namely blanks, analytes, standards, QCs. The tree order will be plate_id, then group, then vial type, then entity, then number of technical replicates.

`plot.PlateObj` *Plotting 96 well plate*

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",
  layoutOverlay = FALSE,
  path = NULL,
  ...
)
```

Arguments

`x`	PlateObj
`color`	character. Coloring variable. Choices: "conc", "group", "dil", "study", "time", "factor", "samples", "arm", "sex", "dose", "route", "matrix". Default is "conc"
`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"
`layoutOverlay`	logical. If TRUE, overlay the plot layout. Default is FALSE
`path`	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_chrom *Plot Chromatogram per Sample for Selected transitions*

Description

This function plots chromatograms for selected transitions per sample.

Usage

```
plot_chrom(
  chrom_res,
  ncol = 2,
  transitions_ids = NULL,
  sample_id,
  integrated = FALSE,
  show_RT = FALSE,
  smoothed = FALSE
)
```

Arguments

chrom_res	ChromRes object
ncol	Number of columns for facet_wrap. If 0, the chromatograms are overlayed in a single plot.
transitions_ids	Vector of transition IDs to plot. If NULL, all transitions are plotted.
sample_id	Sample ID to plot.
integrated	Boolean to show integrated area overlayed
show_RT	Boolean to show RT values
smoothed	Boolean to show smoothed chromatogram

Examples

```
## Not run:
path <- system.file("extdata", "waters_raw_ex", package="PKbioanalysis")
main <- read_chrom(path, method = 1)
plot_chrom(main, ncol = 2, transitions_ids = c(18,19,20), sample_id = 3)
plot_chrom(main, ncol = 3, transitions_ids = c(18,19,20), sample_id = 3)
plot_chrom(main, ncol = 1, transitions_ids = c(18,19,20), sample_id = 3)
plot_chrom(main, ncol = NULL, transitions_ids = c(18,19,20), sample_id = 3)

## End(Not run)
```

---

plot_peak_areas.PeakRes

Plot peak areas

Description

Plot peak areas

Usage

```
plot_peak_areas.PeakRes(
  peaks_res,
  normalize = TRUE,
  blanks = TRUE,
  compounds = NULL,
  analytes = TRUE,
  standards = TRUE,
  QCs = TRUE,
  type = "bar"
)
```

Arguments

peaks_res	PeakRes object
normalize	logical. If TRUE, normalize the peak area by the IS area.
blanks	logical. If TRUE, plot blanks
compounds	numeric vector of compound numbers to include. If NULL, include all compounds
analytes	logical. If TRUE, plot analytes
standards	logical. If TRUE, plot standards
QCs	logical. If TRUE, plot QCs
type	character. Either "bar" or "line"

Value

ggplot2 object

plot_RT.ChromRes *Plotting RT intervals of chromatogram*

Description

Plotting RT intervals of chromatogram

Usage

```
plot_RT.ChromRes(chrom_res)
```

Arguments

chrom_res	ChromRes object

plot_RT.PeakRes *Plot RT*

Description

Plot RT

Usage

```
plot_RT.PeakRes(
  peaks_res,
  normalize = TRUE,
  blanks = TRUE,
  analytes = TRUE,
  standards = TRUE,
  QCs = TRUE,
  facet = FALSE,
  compounds = NULL
)
```

Arguments

peaks_res	PeakRes object
normalize	logical. If TRUE, normalize the peak area by the IS area.
blanks	logical. If TRUE, plot blanks
analytes	logical. If TRUE, plot analytes
standards	logical. If TRUE, plot standards
QCs	logical. If TRUE, plot QCs
facet	logical. If TRUE, facet by compound name
compounds	numeric vector of compound numbers to include. If NULL, include all compounds

Value

ggplot2 object

---

plot_var_pattern *Plot Relationship Between Concentration and CV/SD*

Description

Plot Relationship Between Concentration and CV/SD

Usage

```
plot_var_pattern(df, title = "")
```

Arguments

df	Data frame with columns: stdconc (standardized concentration), cv (coefficient of variation), sdev (standard deviation), Type (e.g., "Estimated", "Observed")
title	Plot title

Author(s)

Omar I. Elashkar

---

precision_per_vial *Precision per vial*

Description

Precision per vial

Usage

```
precision_per_vial(peaks_res, suitability = FALSE)
```

Arguments

peaks_res	PeakRes object
suitability	logical. If TRUE, suitability samples are ignored

Value

ggplot2 object

prefilter_precision_data *Filter data*

Description

Filter data

Usage

```
prefilter_precision_data(
  x,
  type,
  acc_cutoff = 0.2,
  dev_cutoff = 0.2,
  compound_id = NULL
)

## S4 method for signature 'QuantRes'
prefilter_precision_data(
  x,
  type,
  acc_cutoff = 0.2,
  dev_cutoff = 0.2,
  compound_id = NULL
)

## S4 method for signature 'data.frame'
prefilter_precision_data(x, type, acc_cutoff = 0.2, dev_cutoff = 0.2)
```

Arguments

x	Dataframe or QuantRes Object
type	QC, DQC, or Standard
acc_cutoff	Accuracy cutoff. 20% by default
dev_cutoff	Deviation cutoff. 20% by default
compound_id	Compound ID to filter. If NULL, all compounds are considered

Value

Filtered data

Author(s)

Omar I. Elashkar

quant_app *Quantification App*

Description

This function creates a shiny app for quantification after peak integration

Usage

```
quant_app()
```

read_chrom *Read Chromatogram Files*

Description

This function reads chromatogram files from a directory and returns a data frame with the chromatogram data.

Usage

```
read_chrom(dir, format = "waters_raw", method)
```

Arguments

dir	directory for chromatraograms
format	format of the chromatogram files. Options are "waters_raw" and "mzML".
method	LC-MS/MS method ID saved available in the database.

Examples

```
## Not run:
path <- system.file("extdata", "waters_raw_ex", package="PKbioanalysis")
main <- read_chrom(path, method = 1)

## End(Not run)
```

`read_experiment_results` *Read experiment results*

Description

Read experiment results

Usage

```
read_experiment_results(
  x,
  drop_prefix = FALSE,
  vendor = "targetlynx_xml",
  logkey = "Index"
)
```

Arguments

`x`	path to experiment results. See details
`drop_prefix`	logical. If TRUE, drop the prefix from the sample name
`vendor`	vendor name. Currently only "targetlynx_xml" or "targetlynx_csv" are supported.
`logkey`	character. The column name in the targetlynx CSV file that contains the injection sequence or log key. Default is "Index" which is the default column in targetlynx CSV exports, but it can be customized if the user has a different column name for the injection sequence.

Details

Currently only targetlynx XML or CSV exported files are supported.

Value

QuantRes object with the results of the experiment.

`register_plate` *This will save the plate to the database*

Description

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

---

response_to_conc *Convert response to concentration*

Description

Convert response to concentration

Usage

```
response_to_conc(quantres, compound_id, response)
```

Arguments

quantres	QuantRes object
compound_id	character
response	numeric. Must match the response type used in linearity. Either abs_response or rel_response

Value

numeric

---

reverse_predict *Reverse predict concentration from response*

Description

Reverse predict concentration from response

Usage

```
reverse_predict(fit, newdata, intercept)
```

Arguments

fit	lm object
newdata	vector or data frame with response values
intercept	logical. Whether the model has intercept or not

Value

numeric. Estimated concentration

Author(s)

Omar I. Elashkar

---

run_summary *Get Summary of an object*

Description

Get Summary of an object

Usage

```
run_summary(object)

## S3 method for class 'PeakRes'
run_summary(object)
```

Arguments

object	A PeakRes object

---

smooth_chrom *Smooth Chromatogram Peaks*

Description

This function smooths chromatogram peaks using different algorithms.

Usage

```
smooth_chrom(chrom_res, filter = "mean", window = 2, iter = 2)
```

Arguments

chrom_res	ChromRes object
filter	Filter to use. Options are "mean", "median", "savgol", "gaussian"
window	Window size for the filter
iter	Number of iterations. If 0, no smoothing is applied.

---

study_app *bioanalytic_app*

Description

This function creates a shiny app for plate management

Usage

```
study_app()
```

Value

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

---

update_RT *Manually Update Observed RT for either all compounds, all next samples, or single compound and sample*

Description

Update RT for either all compounds, all next samples, or single compound and sample

Usage

```
update_RT(
  chrom_res,
  compound_id,
  sample_id = NULL,
  peak_start,
  peak_end,
  mode = "auto",
  target = "single",
  force = FALSE,
  comment = "",
  flag = FALSE
)
```

Arguments

chrom_res	ChromRes object
compound_id	Compound ID
sample_id	Sample ID (required for "single" and "all_next", must be NULL for "all")
peak_start	Minimum RT value
peak_end	Maximum RT value
mode	Mode of update. Options are "auto", "manual", "ai". Default is "auto"
target	Target of update. Options are "single", "all", "all_next". Default is "single"
force	Force update if previous peak exists. Default is FALSE
comment	Comment for the update. Default is an empty string
flag	Flag the peak after update. Default is FALSE

Details

- target = "single": Updates RT for one compound and sample - target = "all": Updates expected RT for all samples (sets expected bounds) - target = "all_next": Updates RT for specified sample and subsequent samples

All modes affect both observed and expected RT values: - "manual": Sets exact peak bounds, marks as manual - "auto": Auto-detects peaks within bounds - "ai": AI-based peak detection

Value

Updated ChromRes object

Examples

```
## Not run:
update_RT(chrom_res, compound_id = 1, sample_id = 1,
          peak_start = 0.1, peak_end = 1, target = "single")

## End(Not run)
```

---

write_injec_seq *Write injection sequence to database*

Description

Write injection sequence to database

Usage

```
write_injec_seq(injec_seq)
```

Arguments

injec_seq	InjecListObj object

Value

dataframe

[[,MultiPlate-method *Subsetting method for MultiPlate*

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

Index