Package: htrSPRanalysis (via r-universe)

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Type Package

Title Analysis of Surface Plasmon Resonance Data

Version 0.1.0

Description Analysis of Surface Plasmon Resonance (SPR) and Biolayer Interferometry data, with automations for high-throughput SPR. This version of the package fits the 1: 1 binding model, with and without bulkshift. It offers optional local or global Rmax fitting. The user must provide a sample sheet and a Carterra output file in Carterra's current format. There is a utility function to convert from Carterra's old output format. The user may run a custom pipeline or use the provided 'Runscript', which will produce a pdf file containing fitted Rmax, ka, kd and standard errors, a plot of the sensorgram and fits, and a plot of residuals. The script will also produce a .csv file with all of the relevant parameters for each spot on the SPR chip.

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Encoding UTF-8

RoxygenNote 7.3.2

Suggests knitr, rmarkdown, markdown, qpdf

Imports magrittr, readxl, openxlsx, minpack.lm, zoo, stats, gridExtra, grid, parallel, readr, rlang, dplyr, stringr, tidyselect, ggplot2, purrr, forcats, tibble, tidyr

VignetteBuilder knitr

NeedsCompilation no

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Contents

`create_csv` *Create csv file with all fit parameters.*

Description

Create csv file with all fit parameters.

Usage

```
create_csv(processed_input, fits_list)
```

Arguments

`processed_input`	Processed_input as returned by `process_input`
`fits_list`	List of fits as returned by `get_fits`

Value

a data frame with the fit parameters and errors. A csv file is also created using the path name supplied to `process_input`

`create_pdf` *Create pdf file with sensorgrams with fitted curves, residuals, table of fit parameters, and response curves.*

Description

Create pdf file with sensorgrams with fitted curves, residuals, table of fit parameters, and response curves.

Usage

```
create_pdf(processed_input, fits_list, rc_list, plot_list, ...)
```

Arguments

processed_input	Processed_input as returned by process_input
fits_list	List of fits as returned by get_fits
rc_list	List of response curves as returned by get_rc_plots
plot_list	List of plots as returned by get_fitted_plots
...	Arguments passed to the pdf function.

Value

NULL A pdf file is created using the path name supplied to process_input

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get_fits *Get fits of all selected sensorgrams as indicated in the sample information.*

Description

Get fits of all selected sensorgrams as indicated in the sample information.

Usage

```
get_fits(processed_input)
```

Arguments

processed_input	The processed_input object returned by the function process_input.

Value

A list of all fits. The fits are performed using the safely function, so that the list has a $result entry and a $error entry for each item. If $error is NULL, the sensorgram was fit succesfully.

get_fitted_plots *Plot fitted sensorgras and raw data.*

Description

Plot fitted sensorgras and raw data.

Usage

```
get_fitted_plots(processed_input, fits_list)
```

Arguments

processed_input	processed_input as returned by `process_input`
fits_list	List of fits as returned by `get_fits`

Value

list of plots of sensorgrams and fits

get_plots_before_baseline *Plot all raw data that has been selected to be processed (via the* `Incl.` *column in the sample information). No adjustments are made to the data.*

Description

Plot all raw data that has been selected to be processed (via the `Incl.` column in the sample information). No adjustments are made to the data.

Usage

```
get_plots_before_baseline(processed_input)
```

Arguments

processed_input	The list file that is output from the `process_input` function.

Value

A list of all plots that have been selected via the `Incl.` column in sample information

get_rc_plots *Plot response curve. Average RU versus log10 of concentration. Color coded for concentrations selected for fitting.*

Description

Plot response curve. Average RU versus log10 of concentration. Color coded for concentrations selected for fitting.

Usage

```
get_rc_plots(processed_input)
```

Arguments

`processed_input`
: Processed input object as returned from `process_input` function.

Value

list of plots of response curves, indicating the concentrations chosen for fitting

process_input *Process user input files and obtain options for fitting.*

Description

Performs all functions selected in sample information, such as automated dissociation window detection, automated concentration range, automated bulk shift detection and returns a list object with the titration time series, processed sample information, all user inputs directing file outputs and fitting options

Usage

```
process_input(
  sample_sheet_path = NULL,
  data_file_path = NULL,
  output_file_path = NULL,
  output_pdf = NULL,
  output_csv = NULL,
  error_pdf = NULL,
  num_cores = NULL,
  min_allowed_kd = 10^(-5),
  max_iterations = 1000,
  ptol = 10^(-10),
  ftol = 10^(-10),
```

```
  min_RU_tol = 20,
  max_RU_tol = 300
)
```

Arguments

sample_sheet_path	The full path to the sample information file.
data_file_path	The full path to the titration data file.
output_file_path	The full path where output should be stored. This directory needs to exist.
output_pdf	The name of the file for the pdf output.
output_csv	The name of the file for the csv output.
error_pdf	The name of the file for error output.
num_cores	The number of cores to use for parallel processing. The default is(the number of cores detected by `parallel::detectCores()`.
min_allowed_kd	The minimum value for the dissociation constant. The default is 10^(-5).
max_iterations	The maximum number of iterations for curve fitting. The default is 1000.
ptol	Curve fitting parameter. If the proposed changes in parameters is smaller than this value, the optimization is considered converged. The default is 10^(-10)
ftol	Curve fitting parameter. If the squared error between observed and predicted values is smaller than ftol, the optimization is considered converged. The default is 10^(-10)
min_RU_tol	Minimum RU required for dissociation window detection
max_RU_tol	Maximum RU required for dissociation window detection. Also used in curve fitting.

Value

A list object containing the following

expanded_sample_sheet	The sample sheet expanded to include all spots that are represented, expanding the short-hand entries for Position/Block/Channel
sample_info	The expanded sample sheet with only the rows that are to be fit
sample_info_fits	The sample_info without rows that have encountered errors in initial processing
Time	The dataframe whose columns are the Time values for the input titration data. This only includes columns selected for analysis.
RU	The dataframe whose columns are the RU values for the input titration data. Only the columns for the samples to be analyzed are included
correctedRU	The RU dataframe after baseline correction
keep_concentrations	A vector containing the indices of the columns from Time and correctedRU to be used in curve fitting

all_concentrations_values
: A vector containing the concentration values corresponding to the columns of the Time and RU dataframes

incl_concentrations_values
: A vector containing the concentration values corresponding to the Time and correctedRU columns chosen for curve fitting

n_time_points
: The maximum length of titration time series

max_RU_tol
: The maximum RU for dissociation window trimming to be automated

min_RU_tol
: The minimum RU for dissociation window trimming to be automated

min_RU_tol
: The minimum RU for dissociation window trimming to be automated

nwells
: The number of rows in the sample_info dataframe

n_fit_wells
: The number of rows in the sample_info_fits dataframe

ftol
: The ftol parameter passed to the nls.lm function

ptol
: The ptol parameter passed to the nls.lm function

ptol
: The ptol parameter passed to the nls.lm function

output_pdf
: The full pathname for the output pdf file

output_csv
: The full pathname for the output csv file

error_pdf
: The full pathname for the pdf error file. This is where errors in processing can be found.

error_idx_concentrations
: If there is an issue in determining the concentration window for some spots, they will be logged here

Examples

```
# set up file paths for example

 sample_sheet_path <- system.file("extdata",
 "sample_sheet.xlsx", package="htrSPRanalysis")

fn <- paste0("https://gitlab.oit.duke.edu/janice/htrspranalysis/",
        "-/raw/master/inst/extdata/titration_data.xlsx?ref_type=heads")

download.file(fn,
      destfile = paste0(tempdir(),"/titration_data.xlsx"),
      mode = "wb")

data_file_path <- paste0(tempdir(), "/titration_data.xlsx")

# process the input
processed_input <- process_input(sample_sheet_path = sample_sheet_path,
  data_file_path = data_file_path,
   num_cores = 2)
```

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