Package 'HDXBoxeR'

August 24, 2024

Type Package

Title Analysis of Hydrogen-Deuterium Exchange Mass-Spectrometry Data

Version 0.0.2

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Description A protocol that facilitates the processing and analysis of Hydrogen-Deuterium Exchange Mass Spectrometry data using p-value statistics and Critical Interval analysis.
It provides a pipeline for analyzing data from 'HDXExaminer' (Sierra Analytics, Trajan Scientific), automating matching and comparison of protein states through Welch's T-test and the Critical Interval statistical framework.
Additionally, it simplifies data export, generates 'PyMol' scripts, and ensures calculations meet publication standards.
'HDXBoxeR' assists in various aspects of hydrogen-deuterium exchange data analysis, including reprocessing data, calculating parameters, identifying significant peptides, generating plots, and facilitating comparison between protein states.
For details check papers by Hageman and Weis (2019) <doi:10.1021/acs.analchem.9b01325> and Masson et al. (2019) <doi:10.1038/s41592-019-0459-y>.
'HDXBoxeR' citation: Janowska et al. (2024) <doi:10.1093/bioinformatics/btae479>.

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Imports dplyr, graphics, grDevices, RColorBrewer, stats, stringr, tidyr, utils, methods, wrapr

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

VignetteBuilder knitr, rmarkdown

Encoding UTF-8

RoxygenNote 7.2.3

Config/testthat/edition 3

NeedsCompilation no

Repository CRAN

Date/Publication 2024-08-24 07:30:10 UTC

Contents

`all_summary` *Returns full summary table.*

Description

Returns summary data. Function returns: Protein states, timepoints, number of replicates, # peptides, % coveregae, average peptide length and redundancy. backexchange calculations (average and range), Critical interval and standard deviation. Function requires undeuterated and Fully deuterated sets marked in Deut.time as 0s and FD respectively.

Usage

```
all_summary(filepath, replicates = 3, Dfact = 0.85)
```

Arguments

`filepath`	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.
`replicates`	number of replicates. Default set to 3.
`Dfact`	Dfact is the fraction of D/H in the labeling buffer used. Default set up to 0.85

Value

Returns summary table.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- all_summary(file_nm, replicates=3, Dfact=0.85)
```

`arguments_call1` *Returns default arguments for the output_tp functions. States*

Description

Function used as internal function

Usage

```
arguments_call1(filepath)
```

Arguments

`filepath`	input file location

Value

The default arguments to output_tp functions.

`arguments_call2` *Returns default arguments for the output_tp functions. Deut.Time*

Description

Function used as internal function

Usage

```
arguments_call2(filepath, states)
```

Arguments

`filepath`	input file location
`states`	states used

Value

The default arguments to output_tp functions.

`arguments_call3` *Returns default arguments for the output_tp functions. # replicates*

Description

Function used as internal function

Usage

```
arguments_call3(filepath, states, times)
```

Arguments

`filepath`	input file location
`states`	states used
`times`	deuteration times

Value

The default arguments to output_tp functions.

`arg_df` *Returns initially processed data.frame from the export from the HDX-Examiner*

Description

Function used as internal function

Usage

```
arg_df(filepath)
```

Arguments

`filepath`	input file location

Value

Data.frame for further processing

`arg_UN_FD` *Returns initially processed data.frame from the export from the HDX-Examiner*

Description

Function used as internal function

Usage

```
arg_UN_FD(filepath)
```

Arguments

`filepath`	input file location

Value

Data.frame for further processing

`average_timecourse` *Calculates average for time course data.*

Description

Calculates average for time course data.

Usage

```
average_timecourse(filepath)
```

Arguments

`filepath`	filepath to the All_results input file.

Value

data frame with average deuteration uptake data.

ave_timepoint *Returns average value for either uptake of procent data.*

Description

Calculates average of uptake or procent data. Returns data frame with average values. Default for the number of replicates is 3.

Usage

```
ave_timepoint(df, replicates = 3)
```

Arguments

df	output from functions output_tp or output_tp_proc.
replicates	number of replicates used. Default is set to replicates=3

Value

Data.frame with average values

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
ave<-ave_timepoint(df=a) ##if number of replicates is equal 3
ave<-ave_timepoint(df=a, replicates=4) ##if number of replicates is equal 4
```

av_tc *Preparatory function for average plot for timecourses*

Description

Returns plots with average deuteration at each peptide.

Usage

```
av_tc(df, cola)
```

Arguments

df	output from functions output_tp or output_tp or output_tp_proc.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

plots of averages

av_tp *Preparatory function for average plot*

Description

Returns plots with average deuteration at each peptide.

Usage

```
av_tp(df, cola)
```

Arguments

df	output from functions output_tp or output_tp or output_tp_proc.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

plots of averages

backHX_calculations *Summary of backexchange summary*

Description

Returns average and ranges of backexchange. Function calculates as: 1- (m100%-m0%)/N/Dfact. m0% is the non-deuterated peptide centroid mass, m100% is the maximally labeled peptide centroid mass, N is the theoretical number of backbone amides in the peptide and Dfrac is the fraction of D/H in the labeling buffer used. Function requires undeuterated and Fully deuterated sets marked in Deut.time as 0s and FD respectively.

Usage

```
backHX_calculations(filepath, Dfact = 0.85)
```

Arguments

filepath	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.
Dfact	is the fraction of D/H in the labeling buffer used. Default set up to 0.85

Value

Returns summary table for backexchange.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- backHX_calculations(filepath=file_nm, Dfact=0.85)
```

`boxplot_tp` *Plots boxplots for all the averages in the set*

Description

Returns boxplots to compare sets between each other

Usage

```
boxplot_tp(df, replicates = 3, ...)
```

Arguments

`df`	average data frame. Generated using ave_timepoint() function.
`replicates`	number of replicates in sample. Default set to 3.
`...`	inherited boxplot parameters

Value

boxplots for average deuterium uptake per set.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
boxplot_tp(df=a, replicates=3)
```

`CI_2pts` *Global confidence interval treshold from experimental standard deviation for 2 samples.*

Description

Calculation of global confidence interval using approach by: Reliable Identification of Significant Differences in Differential Hydrogen Exchange-Mass Spectrometry Measurements Using a Hybrid Significance Testing Approach Tyler S. Hageman and David D. Weis Analytical Chemistry 2019 91 (13), 8008-8016 DOI: 10.1021/acs.analchem.9b01325 calculations for alpha 0.99

Usage

```
CI_2pts(s1, s2, replicates = 3)
```

Arguments

s1	standard deviation from one sample
s2	standard deviation from seconda sample
replicates	number of replicates. Default set to 3.

Value

treshold for determining significance.

Examples

```
sd1<-data.frame(c(0.1, 0.12, 0.13, 0.09, 0.11, 0.10))
sd2<-data.frame(c(0.18, 0.11, 0.13, 0.08, 0.11, 0.06))
CI_2pts(s1=sd1, s2=sd2, replicates=3)
```

CI_single *Global confidence interval treshold from experimental standard deviation for 1 sample*

Description

Calculation of global confidence interval using approach by: Reliable Identification of Significant Differences in Differential Hydrogen Exchange-Mass Spectrometry Measurements Using a Hybrid Significance Testing Approach Tyler S. Hageman and David D. Weis Analytical Chemistry 2019 91 (13), 8008-8016 DOI: 10.1021/acs.analchem.9b01325 calculations for alpha 0.99

Usage

```
CI_single(s1, replicates = 3)
```

Arguments

s1	standard deviation from one sample
replicates	number of replicates. Default set to 3.

Value

treshold for determining significance.

Examples

```
sd1<-data.frame(c(0.1, 0.12, 0.13, 0.09, 0.11, 0.10))
CI_single(s1=sd1, replicates=3)
```

CI_tc *Critial interval calculation two sets of timecourses*

Description

Preparatory function for calculation of pvalue between sets.

Usage

```
CI_tc(sd_c, sd_v, replicates = 3, pv_cutoff = 0.01)
```

Arguments

sd_c	dataframe of control
sd_v	dataframe for variant
replicates	number of replicates. Default set to 3.
pv_cutoff	pvalue cutoff. Default set to 0.01

Value

Critical interval for 2 sets

CI_tp *Global confidence interval treshold from experimental standard deviation*

Description

Calculation of global confidence interval using approach by for all protein states compared to first state in the data.frame. Reliable Identification of Significant Differences in Differential Hydrogen Exchange-Mass Spectrometry Measurements Using a Hybrid Significance Testing Approach Tyler S. Hageman and David D. Weis Analytical Chemistry 2019 91 (13), 8008-8016 DOI: 10.1021/acs.analchem.9b01325

Usage

```
CI_tp(df, replicates = 3, alpha = 0.01)
```

Arguments

df	standard deviation dataframe.
replicates	number of replicates. Default set to 3.
alpha	significance level. Set as default to 0.01

Value

treshold for determining significance.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tc(file_nm, seq_match=FALSE)
sd<-sd_timepoint(df=a, replicates=3)
CI_tp(df=sd, replicates=3, alpha=0.01 )
CI_tp(sd)
```

---

color_ranges_Blue_Red_heat_map

Returns color pallete from red to blue with number of colors for defined ranges

---

Description

Returns color pallete from red to blue with number of colors for defined ranges

Usage

```
color_ranges_Blue_Red_heat_map(ranges, colors_initial)
```

Arguments

ranges	vector of numbers. Should have the same mumber of positive and negative values and contain 0.
colors_initial	additional color that should be first in the pallette.

Value

color scheme for number

Examples

```
color_ranges_Blue_Red_heat_map(ranges=c(-Inf, -100, -50, 0, 50, 100, Inf), colors_initial="white")
```

color_ranges_Spectral *Returns Spectral pallette with colors matching defined ranges*

Description

Spectral pallette for timecourse data

Usage

```
color_ranges_Spectral(ranges, colors_initial)
```

Arguments

ranges	vector of numbers. Should have the same mumber of positive and negative values and contain 0.
colors_initial	additional color that should be first in the pallette.

Value

color scheme for number

Examples

```
color_ranges_Spectral(ranges=c(-Inf, -100, -50, 0, 50, 100, Inf), colors_initial="white")
```

coverage_residue *Returns coverage per residue*

Description

returns vector with coverage information

Usage

```
coverage_residue(df1, start_col, end_col)
```

Arguments

df1	output from functions output_tp or output_tp_proc.
start_col	number of "Start" column in data.frame
end_col	number of "Start" column in data.frame

Value

vector with coverage per residue

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
coverage_residue(df1=a,start_col=2, end_col=3 )
```

`deuteration_woods_timecourse` *Return woods plots for the timecourse*

Description

All the peptides are plotted based on their uptake.

Usage

```
deuteration_woods_timecourse(
  input_data,
  states,
  replicates = 3,
  ylim = c(0, 120),
  ...
)
```

Arguments

`input_data`	output from function output_tc(..., percent=TRUE)
`states`	states, if missing all states used
`replicates`	replicates
`ylim`	y axis limits
`...`	other parameters

Value

Woods plots for the timecourse

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tc(file_nm, percent=TRUE)
deuteration_woods_timecourse(a)
```

`deuteration_woods_timepoints` *Return woods plots for the timepoints*

Description

All the peptides are plotted based on their uptake.

Usage

```
deuteration_woods_timepoints(
  input_data,
  times,
  replicates = 3,
  cola = NA,
  ylim = c(0, 120),
  ...
)
```

Arguments

`input_data`	output from function output_tp(..., percent=TRUE)
`times`	Deuteration times, if missing all deuteration times used
`replicates`	replicates
`cola`	colors, default NA
`ylim`	y axis limits
`...`	other parameters

Value

Woods plots for the timepoints

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm, percent=TRUE)
deuteration_woods_timepoints(a[1:12,])
```

dif_ave — *Returns data frame with difference of averages between State1 and other states provided.*

Description

Returns average difference data.frame. Sets are compared to the first state in the input file. If other order of the sets is required use Default for the number of replicates is 3.

Usage

```
dif_ave(df)
```

Arguments

df	output from functions output_tp, output_tp_proc, output_tp_states or output_tp_proc_states.

Value

Data.frame with difference values btw control and other protein states.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
pv<-pv_timepoint(df=a) ##if number of replicates is equal 3
pv1<-pv_timepoint(df=a, replicates=3) ##if number of replicates is equal 4
#b<-output_tp_states(file_nm, states=c("4EHP", "State2", "State3" ))
#pv_states<-pv_timepoint(df=b) ### here means of State4, will be compared to State2 and State4
```

dif_tp — *Preparatory function for difference plot*

Description

Returns plots with difference deuteration at each peptide.

Usage

```
dif_tp(df, cola)
```

Arguments

df	output from functions output_tp or output_tp_proc.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

plots of difference in average

`dif_tp_proc` *Preparatory function for difference plot*

Description

Returns plots with difference deuteration at each peptide.

Usage

```
dif_tp_proc(df, cola)
```

Arguments

`df`	output from functions output_tp or output_tp_proc.
`cola`	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

plots of difference in average

`duplicate_sets` *Duplicate set function*

Description

Internal function

Usage

```
duplicate_sets(df)
```

Arguments

`df`	dataframe

Value

duplicate sets

extreme_input_gap *Makes input for Extreme for bimodal analysis.*

Description

Makes input for Extreme for bimodal analysis.

Usage

```
extreme_input_gap(hm_dir, replicates, timepoints, output_path = "NA")
```

Arguments

hm_dir	directory in which all the folders which needs to be processed are
replicates	number of replicates in sample
timepoints	lists timepoints used in experiments.
output_path	directory where the output files will be saved, hm_dir default

Value

Inputs for extreme for all data prepared.

Examples

```
path_to_folders<-system.file("extdata",  package = "HDXBoxeR")

extreme_input_gap(hm_dir =path_to_folders, replicates = 3,
timepoints =c(3, 60, 1800, 72000), output_path=tempdir())
```

extreme_input_undeut *Makes input for Extreme for bimodal analysis.*

Description

If data is missing it returns non-deuterated data in these columns.

Usage

```
extreme_input_undeut(hm_dir, replicates, timepoints, output_path = "NA")
```

Arguments

hm_dir	directory in which all the folders which needs to be processed are
replicates	number of replicates in sample
timepoints	lists timepoints used in experiments.
output_path	directory where output should be written

Value

Inputs for extreme for all data prepared.

Examples

```
path_to_folders<-system.file("extdata",  package = "HDXBoxeR")
extreme_input_undeut(hm_dir=path_to_folders, replicates = 3,
timepoints =c(3, 60, 1800, 72000), output_path=tempdir())
```

---

general_info *Provides summary table for all data.sets.*

Description

Returns data frame sumamrizing general information about the data sets. Function returns: Protein states, timepoints, number of replicates, # peptides, % coveregae, average peptide length and redundancy.

Usage

```
general_info(filepath)
```

Arguments

filepath	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.

Value

Returns summary table.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- general_info(file_nm)
```

getCoords1 *function from plotfunctions package*

Description

Margin coordinates

Usage

```
getCoords1(pos = 1.1, side = 1, input = "p")
```

Arguments

pos	position
side	side of plot
input	plot or figure position

Value

coordinates of margins

heat_map_tc *Plots heat maps for time courses.*

Description

Returns heat map on timecourses with raw data.

Usage

```
heat_map_tc(df, ranges = c(seq(0, 100, by = 10), Inf))
```

Arguments

df	timecourse input
ranges	ranges for coloring scheme. Default set to c(seq(0, 100, by=10), Inf)

Value

heat map for timecourses

heat_map_tp *Preparatory function for heat map*

Description

Returns heat map

Usage

```
heat_map_tp(
  df,
  pv,
  sd,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame. Generated using ave_timepoint() function.
pv	pvalues dataframes calculated using pv_timepoint() function
sd	standard deviation data.frame generated using sd_timepoint function
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

heat map for timepoints

heat_map_tp_maxuptake *Preparatory function for heat map of maximum uptake per residue.*

Description

Returns heat map

Usage

```
heat_map_tp_maxuptake(
  df,
  pv,
  sd,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame. Generated using ave_timepoint() function.
pv	pvalues dataframes calculated using pv_timepoint() function
sd	standard deviation data.frame generated using sd_timepoint function
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

maxiumum uptake heat map for timepoints

---

heat_map_tp_maxuptake_proc

Preparatory function for heat map of maximum procent deuteration per residue.

Description

Returns heat map

Usage

```
heat_map_tp_maxuptake_proc(
  df,
  dfup,
  pv,
  sd,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame for procent deuteration. Generated using ave_timepoint() function.
dfup	average data frame for deuteration uptake. Generated using ave_timepoint() function.
pv	pvalues dataframes calculated using pv_timepoint() function
sd	standard deviation data.frame generated using sd_timepoint function
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

Maximum uptake heat map for timepoints

---

heat_map_tp_proc *Preparatory function for heat map for procent deuteration*

Description

Returns heat map

Usage

```
heat_map_tp_proc(
  df,
  dfup,
  pv,
  sd,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame for procent deuteration. Generated using ave_timepoint() function.
dfup	average data frame for deuteration uptake. Generated using ave_timepoint() function.
pv	pvalues dataframes calculated using pv_timepoint() function
sd	standard deviation data.frame generated using sd_timepoint function
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

heat map for timepoints

`is.nan.data.frame` *Checks for NaN is data.frame*

Description

Function by Hong Ooi; https://stackoverflow.com/questions/18142117/how-to-replace-nan-value-with-zero-in-a-huge-data-frame

Usage

```
## S3 method for class 'data.frame'
is.nan(x)
```

Arguments

`x`	Data frame to be checked for NaN

Value

logical. Returns info if data.frame contains NaNs.

Examples

```
## this function will overwrite the is.nan function that works only on vectors and matrices
df<-data.frame(c(0,NaN), c(1, 2))
is.nan(df)
df[is.nan(df)]<- 0
```

`lab_dif` *Legend for difference in averages plot.*

Description

Returns legend for difference in average plots. Preparatory function.

Usage

```
lab_dif(df, cola)
```

Arguments

`df`	output from functions average difference
`cola`	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

legend for difference in average plot for time points

`lab_dif_proc` *Preparatory function for difference plot for procent deuteration*

Description

Returns legends for plots procent deuteration at each peptide.

Usage

```
lab_dif_proc(df, cola)
```

Arguments

`df`	output from functions output_tp or output_tp_proc.
`cola`	color pallette for different Protein States. As default Paired pallette from RColorBrewer is used.

Value

legends for procent deuteration plots

`lab_vol` *Preparatory function for volcano plot legends*

Description

Returns volcano plots

Usage

```
lab_vol(df, cola)
```

Arguments

`df`	output from functions output_tp
`cola`	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

legends for volcano plots

legend_heat_map *Legend for the heatmaps prep function.*

Description

Returns names for legend for the heatmaps

Usage

```
legend_heat_map(ranges = c(-Inf, seq(-30, 30, by = 10), Inf))
```

Arguments

ranges	ranges that are to be colored in the legend. Default ranges=c(-Inf,seq(-30, 30, by=10), Inf)

Value

legend for the heatmap

legend_heat_map_tc *Legend for the heatmaps for timecourses.*

Description

Returns names for legend for the heatmaps. Extracts names from data.frame

Usage

```
legend_heat_map_tc(df)
```

Arguments

df	generated using output_tcourse()

Value

legend for the heatmap

legend_heat_map_timecourse *Legend for the heatmaps prep function for timecourses.*

Description

Returns names for legend for the heatmaps

Usage

```
legend_heat_map_timecourse(ranges = c(-Inf, seq(0, 100, by = 10), Inf))
```

Arguments

ranges	ranges that are to be colored in the legend. Default ranges=c(-Inf,seq(-30, 30, by=10), Inf)

Value

legend for the heatmap

legend_heat_map_tp *Legend for the heatmaps.Extracts names from data.frame*

Description

Returns names for legend for the heatmaps

Usage

```
legend_heat_map_tp(df)
```

Arguments

df	average data frame. Generated using ave_timepoint() function.

Value

legend for the heatmap

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
legend_heat_map_tp(df=a)
```

legend_heat_map_tp_proc *Legend for the heatmaps percent.Extracts names from data.frame*

Description

Returns names for legend for the heatmaps

Usage

```
legend_heat_map_tp_proc(df)
```

Arguments

df	average data frame.

Value

legend for the heatmap prercent

legend_nm_bottom *Legend, bottom of the plots*

Description

Internal function

Usage

```
legend_nm_bottom(names, cols)
```

Arguments

names	labels
cols	colors

Value

legend at the bottom of the plot

legend_raw_ave *Legend for average plot.*

Description

Returns legend with average plots. Preparatory function.

Usage

```
legend_raw_ave(df, cola)
```

Arguments

df	output from functions output_tp or output_tp_proc.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

legend for average plot for time points

legend_raw_ave_proc *Preparatory function to draw legends for average procent*

Description

Returns legend with average procent deuteration at each peptide.

Usage

```
legend_raw_ave_proc(df, cola)
```

Arguments

df	output from functions output_tp or output_tp_proc.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

legend for average deuteration procent for timepoints

legend_raw_ave_tc *Legend for average deuteration plot for timecourse.*

Description

Returns legend with average plots. Preparatory function.

Usage

```
legend_raw_ave_tc(df, cola)
```

Arguments

df	output from functions output_tp or output_tp_proc.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

legend for average plot for time course

legend_sig_peptides *Legend for the significant peptides*

Description

Returns names for legend for the significant peptides plots.

Usage

```
legend_sig_peptides(ranges = c(-Inf, seq(-30, 30, by = 10), Inf))
```

Arguments

ranges	ranges that are to be colored in the legend. Default ranges=c(-Inf,seq(-30, 30, by=10), Inf)

Value

legend for the heatmap

legend_states_PerD_bottom *Legend, bottom of the plots*

Description

Internal function

Usage

```
legend_states_PerD_bottom(df, cols)
```

Arguments

df	dataframe
cols	colors

Value

legend at the bottom of the plot

legend_tc_bottom *Preparatory function returns legends for the timecourses.*

Description

Preparatory function

Usage

```
legend_tc_bottom(df, cols)
```

Arguments

df	data frame from which names will be extracted
cols	colors to be used in legend

Value

legend at the bottom of the plot

nb_exch_deut *Number of exchangeable protons*

Description

Provides a vector with number of exchangeable protons, calculated from the input table. Number of protons calculated as peptide_length - 2 - number of Prolines in the peptide that are not in the first position

Usage

```
nb_exch_deut(df)
```

Arguments

df	standard deviation from one sample

Value

vector with number of exchangeable protons

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
nb_exch_deut(a)
```

nm_states *Lists names of states in data sets*

Description

Returns vector with name of states used for choosing states for input functions generation.

Usage

```
nm_states(filepath)
```

Arguments

filepath	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.

Value

list of Protein States.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
names_states<- nm_states(file_nm)
```

`output_FD` *Prepares output for HDX-MS Full deuteration data*

Description

Returns a data frame for Full deuteration set

Usage

```
output_FD(filepath)
```

Arguments

`filepath`	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.

Value

data frame with reorganized data where in columns is uptake data for Protein States.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<-output_FD(file_nm)
```

`output_FD_proc` *Prepares output for HDX-MS Full deuteration data for procent deuteration.*

Description

Returns a data frame for Full deuteration set

Usage

```
output_FD_proc(filepath)
```

Arguments

`filepath`	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.

Value

data frame with reorganized data where in columns is procent deuteration for Protein States.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_FD_proc(file_nm)
```

`output_prep` *Prepares output with HDX-MS data for publications*

Description

Format prepared based of example from: Masson, G.R., Burke, J.E., Ahn, N.G. et al. Recommendations for performing, interpreting and reporting hydrogen deuterium exchange mass spectrometry (HDX-MS) experiments. Nat Methods 16, 595–602 (2019). https://doi.org/10.1038/s41592-019-0459-y It generates csv file in format ready for publication of the data.

Usage

```
output_prep(filepath, output_name, states, replicates, times, percent = FALSE)
```

Arguments

`filepath`	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.
`output_name`	Name of output file. It has to be csv file
`states`	function allows to choose what states should be used for analysis. Default all states are used.
`replicates`	number of replicates to be used in analysis. The function takes number of replicates up to specified number. If no argument provided number maximal common number of replicates it used.
`times`	lists the deuteration times to be used in analysis. Default all states used.
`percent`	return either uptake or percent deuteration, default=FALSE, return uptake

Value

Returns&saves data.frame in format that is accepted for the publications.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
output_prep(filepath=file_nm, output_name=tempfile())
```

output_tc *Prepares output for HDX-MS for the deuteration uptake or percent deuteration for the time courses.*

Description

Returns a data frame organized for additional analysis. In columns are deuteration uptake or percent deuteration data for the given protein states. Function allows for writing csv with data, matching sequences of peptide. Protein.States, Deut.times, or number of replicates can be specified.

Usage

```
output_tc(
  filepath,
  replicates,
  states,
  times,
  seq_match = FALSE,
  csv = "NA",
  percent = FALSE
)
```

Arguments

filepath	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.
replicates	number of replicates to be used in analysis. The function takes number of replicates up to specified number. If no argument provided number maximal common number of replicates it used.
states	function allows to choose what states should be used for analysis. Default all states are used.
times	lists the deuteration times to be used in analysis. Default all states used.
seq_match	Flag allows to choose if the peptide sequences should be matched between states. seq_match=FALSE signifies no sequence matching, seq_match=TRUE states that the sequences are matched between the sets.
csv	Flag allowing saving the output as csv. With default csv="NA", data is not saved. If csv output is desided, provide output name.
percent	Flag allowing to choose output as deteuration uptake (FALSE) or percent deuteration (TRUE). Default deuteration uptake.

Value

data frame with reorganized data where in columns is the deuteration uptake for Protein States.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tc(filepath=file_nm) ###all default parameters used

# all possible flags listed & percent deuteration output,
#with sequences matching for protein states.

a<-output_tc(filepath=file_nm, replicates=3, states=c("bound", "Unbound"),
times=c("3.00s", "72000.00s"), seq_match=TRUE, csv="NA", percent=TRUE)
```

`output_tp` *Prepares output for HDX-MS for the deuteration uptake or percent deuteration for the time points.*

Description

Returns a data frame organized for additional analysis. In columns are deuteration uptake or percent deuteration data for the given protein states. Function allows for writing csv with data, matching sequences of peptide. Protein.States, Deut.times, or number of replicates can be specified.

Usage

```
output_tp(
  filepath,
  replicates,
  states,
  times,
  seq_match = FALSE,
  csv = "NA",
  percent = FALSE
)
```

Arguments

`filepath`	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.
`replicates`	number of replicates to be used in analysis. The function takes number of replicates up to specified number. If no argument provided number maximal common number of replicates it used.
`states`	function allows to choose what states should be used for analysis. Default all states are used.
`times`	lists the deuteration times to be used in analysis. Default all states used.
`seq_match`	Flag allows to choose if the peptide sequences should be matched between states. seq_match=FALSE signifies no sequence matching, seq_match=T states that the sequences are matched between the sets.

csv	Flag allowing saving the output as csv. With default csv="NA", data is not saved. If csv output is desided, provide output name.
percent	Flag allowing to choose output as deteuration uptake (FALSE) or percent deuteration (TRUE). Default deuteration uptake.

Value

data frame with reorganized data where in columns is the deuteration uptake for Protein States.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(filepath=file_nm) ###all default parameters used


# all possible flags listed & percent deuteration output,
# with sequences matching for protein states.

a<-output_tp(filepath=file_nm, replicates=3, states=c("bound", "Unbound"),
times=c("3.00s", "72000.00s"), seq_match=TRUE, csv="NA", percent=TRUE)
```

---

output_UD *Prepares output for HDX-MS Undeuterated sample data.*

Description

Returns a data frame for Full deuteration set

Usage

```
output_UD(filepath)
```

Arguments

filepath	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.

Value

data frame with reorganized data where in columns is uptake data for Protein States.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_UD(file_nm)
```

output_UD_proc *Prepares output for HDX-MS Undeuterated data for procent deuteration.*

Description

Returns a data frame for Undeuterated control set

Usage

```
output_UD_proc(filepath)
```

Arguments

filepath	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.

Value

data frame with reorganized data where in columns is procent deuteration for Protein States.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_UD_proc(file_nm)
```

pallette_legend *Color scheme using heatmap. Legend Extracts names from data.frame*

Description

Returns names for legend for the heatmaps

Usage

```
pallette_legend(col_pallette)
```

Arguments

col_pallette	pallette to be used in the heat map

Value

legend for the heatmap

pallette_ll *Color scheme using heatmap. Legend extracts names from data frame*

Description

Returns names for legend for the heatmaps

Usage

```
pallette_ll(pallette, lab)
```

Arguments

pallette	pallette to be used in the heat map
lab	labels to be used in pallette

Value

legend for the heatmap

peptide_pv_tp *Preparatory function for significant peptide plots*

Description

Returns plot where significant peptides are colored in blue-red scheme.

Usage

```
peptide_pv_tp(
  df,
  pv,
  sd,
  nb_row,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame. Generated using ave_timepoint() function.
pv	pvalues dataframes calculated using pv_timepoint() function
sd	standard deviation data.frame generated using sd_timepoint function
nb_row	number of peptides in each row. Plotting parameter.
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

plot with peptides which are significantly different between sets.

---

peptide_pv_tp_proc *Preparatory function for showing peptides with significant differences between sets.*

Description

Returns plot where significantly different peptides are colored in blue-red scheme.

Usage

```
peptide_pv_tp_proc(
  df,
  dfup,
  pv,
  sd,
  nb_row = 100,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame for procent deuteration. Generated using ave_timepoint() function.
dfup	average data frame for deuteration uptake. Generated using ave_timepoint() function.
pv	pvalues dataframes calculated using pv_timepoint() function
sd	standard deviation data.frame generated using sd_timepoint function
nb_row	number of peptides in each row. Plotting parameter.
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

plot with peptides which are significantly different between sets.

`plots_av_tcourse` *Generates average deuteration plot for the time-course.*

Description

Returns plots with average deuteration at each peptide.

Usage

```
plots_av_tcourse(df, replicates = 3, cola)
```

Arguments

`df`	output from functions output_tcourse or output_tcourse_proc.
`replicates`	number of replicates in set as default set to 3.
`cola`	color pallette for different Protein States. As default Paired pallette from RColorBrewer is used.

Value

average deuteration plots

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tc(file_nm)
plots_av_tcourse(df=a, replicates=3, cola=c(1:4))
plots_av_tcourse(df=a)
```

`plots_av_tp` *Returns average deuteration plot for timepoints in the data frame*

Description

Returns plots with average deuteration at each peptide.

Usage

```
plots_av_tp(df, replicates = 3, cola)
```

Arguments

df	output from functions output_tp or output_tp_proc.
replicates	number of replicates in set as default set to 3.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

average deuteration plots

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
plots_av_tp(df=a, replicates=3, cola=c(1:4))
plots_av_tp(df=a)
```

---

plots_av_tp_proc *Returns average procent deuteration plot for time points*

Description

Returns plots with average procent deuteration at each peptide.

Usage

```
plots_av_tp_proc(df, replicates = 3, cola)
```

Arguments

df	output from functions output_tp_proc.
replicates	number of replicates in set as default set to 3.
cola	color pallette for different Protein States. As default Paired pallette from RColorBrewer is used.

Value

average deuteration plots

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm, percent=TRUE)
plots_av_tp_proc(df=a, replicates=3, cola=c(1:4))
plots_av_tp_proc(df=a)
```

plots_diff_tp — *Returns difference in average plot for timepoints in the data frame*

Description

Returns plots with difference in avarage for each peptide.

Usage

```
plots_diff_tp(df, replicates = 3, cola)
```

Arguments

df	output from functions output_tp or output_tp_proc.
replicates	number of replicates in set as default set to 3.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

plots of difference of averages

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
plots_diff_tp(df=a, replicates=3, cola=c(1:4))
plots_diff_tp(df=a)
```

plots_diff_tp_proc — *Returns difference in average procent deuteration plot for timepoints in the data frame*

Description

Returns plots with difference in procent deuteration for each peptide.

Usage

```
plots_diff_tp_proc(df, replicates = 3, cola)
```

Arguments

df	output from functions output_tp_proc.
replicates	number of replicates in set as default set to 3.
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

plots of difference of average procent deuteration

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm, percent=TRUE)
plots_diff_tp_proc(df=a, replicates=3, cola=c(1:4))
plots_diff_tp_proc(df=a)
```

`plots_vol_tp` *Returns volcano plots for timepoints in the data frame*

Description

Returns volcano plots for each peptide. Critical interval is calculated according to #' Reliable Identification of Significant Differences in Differential Hydrogen Exchange-Mass Spectrometry Measurements Using a Hybrid Significance Testing Approach Tyler S. Hageman and David D. Weis Analytical Chemistry 2019 91 (13), 8008-8016 DOI: 10.1021/acs.analchem.9b01325 calculations for alpha 0.99 pvalues calculated using Welch t-test.

Usage

```
plots_vol_tp(df, replicates = 3, pv_cutoff = 0.01, cola)
```

Arguments

`df`	output from functions output_tp
`replicates`	number of replicates in set as default set to 3.
`pv_cutoff`	p-value cutoff here set up to 0.01
`cola`	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

volcano plots

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
plots_vol_tp(df=a, replicates=3, cola=c(1:4), pv_cutoff=0.01 )
plots_vol_tp(df=a, pv_cutoff=0.05)
```

plot_heat_map_max_uptake_tp *Plots heat maps for maximum uptake per residue.*

Description

Returns heat map with maximum uptake per residue.

Usage

```
plot_heat_map_max_uptake_tp(
  df,
  replicates = 3,
  mar_x = 3.5,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01
)
```

Arguments

df	average data frame. Generated using ave_timepoint() function.
replicates	number of replicates in sample. Default set to 3.
mar_x	margin x width. Default=3.5
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01

Value

heat map for maximum uptake per residue

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
plot_heat_map_max_uptake_tp(df=a, replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf) )
plot_heat_map_max_uptake_tp(df=a)
```

plot_heat_map_max_uptake_tp_proc *Plots heat maps for maximum procent deuteration per residue.*

Description

Returns heat map with maximum precent_deuteration per residue.

Usage

```
plot_heat_map_max_uptake_tp_proc(
  input_proc,
  input_up,
  mar_x = 3.5,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

input_proc	Dataframe with organized procent deuteration data. Input generated using output_tp_proc() function.
input_up	Dataframe with organized deuteration uptake. Input generated using output_tp() function.
mar_x	margin x width. Default=3.5
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

heat map for average uptake per residue for significant peptides.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a_up<- output_tp(file_nm)
a_proc<- output_tp(file_nm, percent=TRUE)
plot_heat_map_max_uptake_tp_proc(input_proc=a_proc, input_up=a_up, replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf) )
plot_heat_map_max_uptake_tp_proc(input_proc=a_proc, input_up=a_up)
```

plot_heat_map_tc *Plots heat maps for time courses.*

Description

Returns heat map on timecourses with raw data.

Usage

```
plot_heat_map_tc(
  df,
  replicates = 3,
  mar_x = 3.5,
  ranges = c(-Inf, seq(0, 100, by = 10), Inf)
)
```

Arguments

df	output from function output_tcourse
replicates	number of replicates in sample. Default set to 3.
mar_x	margin x width. Default=3.5
ranges	ranges for coloring scheme. Default set to c(seq(0, 100, by=10), Inf)

Value

heat map for time courses

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tc(file_nm)
plot_heat_map_tc(df=a, replicates=3, ranges=c(seq(0, 100, by=5), Inf))
plot_heat_map_tc(df=a)
```

plot_heat_map_tp *Plots heat maps for significant peptides.*

Description

Returns heat map with average values for significant uptake per residue.

Usage

```
plot_heat_map_tp(
  df,
  mar_x = 3.5,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame. Generated using ave_timepoint() function.
mar_x	margin x width. Default=3.5
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

heat map for average uptake per residue for significant peptides.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
plot_heat_map_tp(df=a, replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf) )
plot_heat_map_tp(df=a)
```

---

plot_heat_map_tp_proc *Plots heat maps for significant peptides.*

Description

Returns heat map with average values for significant uptake per residue.

Usage

```
plot_heat_map_tp_proc(
  input_proc,
  input_up,
  mar_x = 3.5,
  ranges = c(-Inf, -3, -2, -1, 0, 1, 2, 3, Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

input_proc	Dataframe with organized procent deuteration data. Input generated using output_tp_proc() function.
input_up	Dataframe with organized deuteration uptake. Input generated using output_tp() function.
mar_x	margin x width. Default=3.5
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

heat map for average uptake per residue for significant peptides.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a_up<- output_tp(file_nm)
a_proc<- output_tp(file_nm, percent=TRUE)
plot_heat_map_tp_proc(input_proc=a_proc, input_up=a_up, replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf) )
plot_heat_map_tp_proc(input_proc=a_proc, input_up=a_up)
```

---

plot_peptide_sig_tp *Significant peptide plots.*

Description

Returns plot where significant peptides are colored in blue-red scheme.

Usage

```
plot_peptide_sig_tp(
  df1,
  replicates = 3,
  nb_pep_row = 100,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01
)
```

Arguments

df1	average data frame. Generated using ave_timepoint() function.
replicates	number of replicates in sample. Default set to 3.
nb_pep_row	number of peptides in each row. Plotting parameter. Default set to 100.
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01

Value

plot with peptides which are significantly different between sets.

`plot_peptide_sig_tp_proc` *Draws peptides with significant difefrences between sets.*

Description

Returns plot where significant peptides are colored in blue-red scheme.

Usage

```
plot_peptide_sig_tp_proc(
  input_proc,
  input_up,
  nb_pep_row = 100,
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

`input_proc`	Dataframe with organized procent deuteration data. Input generated using output_tp_proc() function.
`input_up`	Dataframe with organized deuteration uptake. Input generated using output_tp() function.
`nb_pep_row`	number of peptides in each row. Plotting parameter. Default set to 100.
`ranges`	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
`pv_cutoff`	p-value cutoff here set up to 0.01
`replicates`	number of replicates in sample. Default set to 3.

Value

plot with peptides which are significantly different between sets.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a_up<- output_tp(file_nm)
a_proc<- output_tp(file_nm, percent=TRUE)
plot_peptide_sig_tp_proc(input_proc=a_proc, input_up=a_up, replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf), nb_pep_row=40 )
```

pl_gen_ch2 *Prepares the plot window for the woods functions*

Description

Internal function

Usage

```
pl_gen_ch2(df, ddlab = 1, ...)
```

Arguments

df	dataframe
ddlab	label
...	other

Value

Plot window

pl_gen_uptake *Prepares the plot window for the woods functions*

Description

Internal function

Usage

```
pl_gen_uptake(df, timepoints, ddlab = 1, ...)
```

Arguments

df	dataframe
timepoints	deuteration times used
ddlab	label
...	other

Value

Plot window

ppar *Preparation of figure window.*

Description

Prepares a plotting window with specified margins with specific number of figure row and columns.

Usage

```
ppar(mfrow2)
```

Arguments

mfrow2	mfrow: number of Multiple Figures (use ROW-wise).

Value

modified par function with adjusted parameters

Examples

```
ppar(c(2,1))
```

pparLM *Preparation of figure window. small margins*

Description

Prepares a plotting window with specified margins with specific number of figure row and columns.

Usage

```
pparLM(mfrow2)
```

Arguments

mfrow2	mfrow: number of Multiple Figures (use ROW-wise).

Value

modified par function with adjusted parameters

Examples

```
pparLM(c(2,1))
```

ppar_bottom_legend *Preparation of figure window with area for figure at the bottom.*

Description

Prepares a plotting window with specified margins with specific number of figure row and columns.

Usage

```
ppar_bottom_legend(mfrow2)
```

Arguments

mfrow2	mfrow: number of Multiple Figures (use ROW-wise).

Value

modified par function with adjusted parameters

Examples

```
ppar_bottom_legend(c(2,3))
```

ppar_wider *Preparation of figure window with more area on west side of plot.*

Description

Prepares a plotting window with specified margins with specific number of figure row and columns.

Usage

```
ppar_wider(mfrow2)
```

Arguments

mfrow2	mfrow: number of Multiple Figures (use ROW-wise).

Value

default plotting window

Examples

```
ppar_wider(c(2,1))
```

`prep_timecourse_plot_ave` *Prepares function for plotting averages in timecourse*

Description

Preparatory function

Usage

```
prep_timecourse_plot_ave(control_df, variant_df, replicates = 3)
```

Arguments

`control_df`	dataframe of control
`variant_df`	dataframe for variant
`replicates`	number of replicates. Default set to 3.

Value

dataframes with matched peptides in time course

`prep_timecourse_plot_sd` *Prepares function for Critical interval for timecourses*

Description

Preparatory function

Usage

```
prep_timecourse_plot_sd(
  control_df_up,
  variant_df_up,
  replicates = 3,
  pv_cutoff = 0.01
)
```

Arguments

`control_df_up`	dataframe of control
`variant_df_up`	dataframe for variant
`replicates`	number of replicates. Default set to 3.
`pv_cutoff`	cut off of pvalue used in calculation of critical interval. Default set to 0.01

Value

Critial interval for all sets

`pv_timecourse` *pvalue calculation between two sets of the data at certain timepoint*

Description

Preparatory function for calculation of pvalue between sets.

Usage

```
pv_timecourse(df_c, df_v, replicates = 3)
```

Arguments

`df_c`	dataframe of control
`df_v`	dataframe for variant
`replicates`	number of replicates. Default set to 3.

Value

pvalue comparisons between two sets.

`pv_timepoint` *Calculation of pvalue between first protein state and any other state from all_states file*

Description

Compares means of sets of uptake data and return dataframe with pvalues. Welch t.test is used for analysis. Sets are compared to the first state in the input file. If other order of the sets is required use Default for the number of replicates is 3.

Usage

```
pv_timepoint(df, replicates = 3)
```

Arguments

`df`	output from functions output_tp or output_tp_proc.
`replicates`	number of replicates used. Default is set to replicates=3

Value

Data.frame with p-values

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
pv<-pv_timepoint(df=a) ##if number of replicates is equal 3
# pv1<-pv_timepoint(df=a, replicates=4) ##if number of replicates is equal 4
#b<-output_tp_states(file_nm, states=c("State4", "State2", "State3" ))
#pv_states<-pv_timepoint(df=b) ### here means of State4, will be compared to State2 and State4
```

---

pymol_script_average_residue

Writes a text files with pymol scripts to list significant residues.

Description

Function write a script that can be used in pymol to color structure. Number of colors and corresponding to them ranges can be defined by user. Residues are being colored by average uptake values from the significant peptides per residues.

Usage

```
pymol_script_average_residue(
  df,
  path = "",
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	output from functions output_tp
path	output folder location
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

pymol script with residues colored based on average of uptake per residue.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
pymol_script_average_residue(df=a, replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf), path=tempdir() )
pymol_script_average_residue(df=a,  path=tempdir())
```

`pymol_script_significant_peptide` *Writes a text files with pymol scripts to list significant peptides*

Description

Function write a script that can be used in pymol to color structure. Number of colors and corresponding to them ranges can be defined by user.

Usage

```
pymol_script_significant_peptide(
  df,
  path = "",
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3,
  order.pep = TRUE
)
```

Arguments

`df`	output from functions output_tp
`path`	location where the scripts will be saved
`ranges`	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
`pv_cutoff`	p-value cutoff here set up to 0.01
`replicates`	number of replicates in sample. Default set to 3.
`order.pep`	flag allowing to either order peptide acccording to the peptide length (default), or to position in the protein sequence.

Value

pymol script with colors assigned per peptide

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
pymol_script_significant_peptide(df=a, replicates=3, path=tempdir(), pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf), order.pep=TRUE )
pymol_script_significant_peptide(df=a, path=tempdir())
```

---

pymol_script_significant_peptide_proc

Writes a text files with pymol scripts to list significant peptides

---

Description

Function write a script that can be used in pymol to color structure. Number of colors and corresponding to them ranges can be defined by user.

Usage

```
pymol_script_significant_peptide_proc(
  input_proc,
  input_up,
  path = "",
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3,
  order.pep = TRUE
)
```

Arguments

input_proc	Dataframe with organized procent deuteration data. Input generated using output_tp(, percent=T) function.
input_up	Dataframe with organized deuteration uptake. Input generated using output_tp() function.
path	location where the Pymol scripts will be saved
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.
order.pep	flag allowing to either order peptide acccording to the peptide length (default), or to position in the protein sequence.

Value

pymol script with colors assigned per peptide

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a_up<- output_tp(file_nm)
a_proc<- output_tp(file_nm, percent=TRUE)
pymol_script_significant_peptide_proc(input_proc=a_proc,
input_up=a_up,  path=tempdir(),replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf), order.pep=TRUE)
```

---

pymol_script_significant_residue

Writes a text files with pymol scripts to list significant residues.

Description

Function write a script that can be used in pymol to color structure. Number of colors and corresponding to them ranges can be defined by user. Residues are being colored by maximum uptake from significant peptides per residues.

Usage

```
pymol_script_significant_residue(
  df,
  path = "",
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

df	average data frame. Generated using ave_timepoint() function.
path	location where the Pymol scripts will be saved
ranges	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
pv_cutoff	p-value cutoff here set up to 0.01
replicates	number of replicates in sample. Default set to 3.

Value

pymol script with colors assigned per residues by maximum uptake per residue

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
pymol_script_significant_residue(df=a, path=tempdir(), replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf) )
pymol_script_significant_residue(df=a, path=tempdir())
```

`pymol_script_significant_residue_proc` *Writes a text files with pymol scripts to list significant residues.*

Description

Function write a script that can be used in pymol to color structure. Number of colors and corresponding to them ranges can be defined by user. Residues are colored by average procent_deuteration from the significant peptides per residues.

Usage

```
pymol_script_significant_residue_proc(
  input_up,
  input_proc,
  path = "",
  ranges = c(-Inf, seq(-30, 30, by = 10), Inf),
  pv_cutoff = 0.01,
  replicates = 3
)
```

Arguments

`input_up`	Dataframe with organized deuteration uptake. Input generated using output_tp() function.
`input_proc`	Dataframe with organized procent deuteration data. Input generated using output_tp_proc() function.
`path`	location where the Pymol scripts will be saved
`ranges`	ranges for coloring scheme. Default set to c(-Inf, seq(-30, 30, by=10), Inf)
`pv_cutoff`	p-value cutoff here set up to 0.01
`replicates`	number of replicates in sample. Default set to 3.

Value

pymol script with residues colored based on average of procent deuteration per residue.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a_up<- output_tp(file_nm)
a_proc<- output_tp(file_nm, percent=TRUE)
pymol_script_significant_residue_proc(input_proc=a_proc,
input_up=a_up, path=tempdir(), replicates=3, pv_cutoff=0.01,
ranges=c(-Inf,-40, -30,-20,-10, 0,10, 20,30,40, Inf))
```

---

pymol_str *Preparatory function writing pymol scripts*

Description

Function rearrange vector to string by adding + sign between the numbers.

Usage

```
pymol_str(ind1)
```

Arguments

ind1	vector of numbers (residues)

Value

string with + as a separator.

Examples

```
res<-c(1,5, 19, 100, 109)
pymol_str(res)
```

---

qpcr.cbind.na *Hidden function from qpcR package, typical usage as qpcR:::cbind.na*

Description

Combine data of unequal row length avoiding repetition or errors by filling with NAs. In contrast to classical cbind, cbind.na can be used to combine data such as

Usage

```
qpcr.cbind.na(..., deparse.level = 1)
```

Arguments

...	vectors
deparse.level	set to 1 as default

Value

data frame with NA

Examples

```
qpcr.cbind.na(1:10, 1:3)
```

---

ranges_function *Gives ranges for the averages*

Description

Function used as internal function to get ranges in the function.

Usage

```
ranges_function(df_ave, values_df)
```

Arguments

df_ave	average per residues
values_df	data frame with values.

Value

ranges per set

---

ranges_function_tc *Gives ranges for the averages for time course analysis*

Description

Function used as internal function to get ranges in the function.

Usage

```
ranges_function_tc(df_ave, values_df)
```

Arguments

df_ave	average per residues
values_df	data frame with values.

Value

ranges per set

---

rbind_na *bind non equal row*

Description

kmezhoud/canceR: A Graphical User Interface for accessing and modeling the Cancer Genomics Data of MSKCC https://rdrr.io/github/kmezhoud/canceR/src/R/rbind.na.R

Usage

```
rbind_na(..., deparse.level = 1)
```

Arguments

...	(generalized) vectors or matrices.
deparse.level	integer controlling the construction of labels in the case of non-matrix-like arguments (for the default method): deparse.level = 0 constructs no labels; the default, deparse.level = 1 or 2 constructs labels from the argument names.

Value

a data frame with merged rows

Examples

```
row1 <- c("a","b","c","d")
row2 <- c("A", "B", "C")
row3 <- rbind_na(row1, row2)
```

reset_par *Reset plotting window parameters to default*

Description

function by Farid Cheraghi, https://stackoverflow.com/questions/9292563/reset-the-graphical-parameters-back-to-default-values-without-use-of-dev-off function resets plotting window parameters

Usage

```
reset_par()
```

Value

default plotting window parameters

Examples

```
reset_par()
```

robot_2states_indexes *Returns a robot plot for selected peptides for 2 protein states.*

Description

Modification of butterfly plot. x axis residues. y axis % deuteration for one variant above the axis and for second peptide below the axis. Peptides are compared between the sets for the significance change between sets. If there is significant change beteween sets peptides are plotted for all timepoints. Significanty different timepoints for the peptides are colored. Peptides ranges are plotted as a line at corresponding % deuteration values.

Usage

```
robot_2states_indexes(
  thP,
  th,
  indexes,
  states,
  replicates = 3,
  pvalue = 0.01,
  ylim,
  xlim,
  CI_factor = 1
)
```

Arguments

thP	output of output_tcourse_proc() function. Raw data for procent deuteration for time courses
th	output of output_tcourse() function. Raw data for uptake deuteration for time courses
indexes	indexes of peptides to be drawn.
states	Need to choose only two protein states
replicates	number of replicates in sample. Default set to 3.
pvalue	p-value cutoff here set up to 0.01
ylim	y-axis range
xlim	x-axis range. Set as default from max and minimum residues for the protein
CI_factor	Multiplication factor for Critical Interval. Allows for more restrictive selection of Critial interval.

Value

Robot maps for timecourses for 2 protein states and selected indexes.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
tm_df<-output_tc(filepath=file_nm)
tmP_df<-output_tc(filepath=file_nm, percent=TRUE)
names_states<- nm_states(file_nm) ### returns states names
ind1<-robot_indexes(thP = tmP_df, th=tm_df, pvalue=0.001, CI_factor=3, states=names_states[1:2])
robot_2states_indexes(thP = tmP_df, th=tm_df,
 states=names_states[1:2],indexes =ind1, pvalue=0.001, CI_factor=3)
```

---

robot_indexes *Returns indexes for peptides with significant difference between two sets*

Description

Function to help decide which peptides will be drawn on Robot plots.

Usage

```
robot_indexes(thP, th, replicates = 3, pvalue = 0.01, states, CI_factor = 1)
```

Arguments

thP	output of output_tcourse_proc() function. Raw data for procent deuteration for time courses
th	output of output_tcourse() function. Raw data for uptake deuteration for time courses
replicates	number of replicates in sample. Default set to 3.
pvalue	p-value cutoff. Default set up to 0.01
states	Protein states from the set. As default all states are chosen.
CI_factor	Multiplication factor for Critical Interval. Allows for more restrictive selection of Critial interval.

Value

Returns indexes of significant peptides

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
tm_df<-output_tc(filepath=file_nm)
tmP_df<-output_tc(filepath=file_nm, percent=TRUE)

 # more restictive peptide selection
robot_indexes(thP = tmP_df, th=tm_df, pvalue=0.01, CI_factor=1.5)
```

---

robot_indexes_df *Returns dataframe with peptides which exhibit significant difference between two sets*

Description

Function to help decide which peptides will be drawn on Robot plots.

Usage

```
robot_indexes_df(thP, th, replicates = 3, pvalue = 0.01, states, CI_factor = 1)
```

Arguments

thP	output of output_tcourse_proc() function. Raw data for procent deuteration for time courses
th	output of output_tcourse() function. Raw data for uptake deuteration for time courses
replicates	number of replicates in sample. Default set to 3.
pvalue	p-value cutoff. Default set up to 0.01
states	Protein states from the set. As default all states are chosen.
CI_factor	Multiplication factor for Critical Interval. Allows for more restrictive selection of Critial interval.

Value

Returns dataframe listing peptides that are significantly different between sets.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
tm_df<-output_tc(filepath=file_nm)
tmP_df<-output_tc(filepath=file_nm, percent=TRUE)

# more restictive peptide selection
robot_indexes_df(thP = tmP_df, th=tm_df, pvalue=0.01, CI_factor=1.5)
```

---

robot_plot_All *Returns a robot plot for comparisons of the timepoints samples*

Description

Modification of butterfly plot. x axis residues. y axis % deuteration for one variant above the axis and for second peptide below the axis. Peptides are compared between the sets for the significance change between sets. If there is significant change beteween sets peptides are plotted for all timepoints. Significanty different timepoints for the peptides are colored. Peptides ranges are plotted as a line at corresponding % deuteration values.

Usage

```
robot_plot_All(
  thP,
  th,
  replicates = 3,
  pv_cutoff = 0.01,
  states,
  CI_factor = 1
)
```

Arguments

thP	output of output_tcourse_proc() function. Raw data for procent deuteration for time courses
th	output of output_tcourse() function. Raw data for uptake deuteration for time courses
replicates	number of replicates in sample. Default set to 3.
pv_cutoff	p-value cutoff here set up to 0.01
states	Protein states from the set. As default all states are chosen.
CI_factor	Multiplication factor for Critical Interval. Allows for more restrictive selection of Critial interval.

Value

Robot maps for timecourses

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
tm_df<-output_tc(filepath=file_nm)
tmP_df<-output_tc(filepath=file_nm, percent=TRUE)
robot_plot_All(thP = tmP_df, th=tm_df, pv_cutoff=0.001)

# more restrictive peptide selection
robot_plot_All(thP = tmP_df, th=tm_df, pv_cutoff=0.001, CI_factor=3)
```

---

sd_timecourse *Returns standard deviation for uptake data for timecourses.*

Description

Calculates standard deviation for timecourse data.

Usage

```
sd_timecourse(filepath)
```

Arguments

filepath	filepath to the All_results input file.

Value

Data.frame with standard deviation.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
sd_timecourse(filepath=file_nm)
```

sd_timecourse_proc *Returns standard deviation for percent deuteration data for time-courses.*

Description

Calculates standard deviation for time course data.

Usage

```
sd_timecourse_proc(filepath)
```

Arguments

filepath	filepath to the All_results input file.

Value

Data.frame with standard deviation.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
sd_timecourse(filepath=file_nm)
```

sd_timepoint *Returns standard deviation for dataframe.*

Description

Calculates standard deviation for the number of replicates in the function.

Usage

```
sd_timepoint(df, replicates = 3)
```

Arguments

df	output from functions output_tp or output_tp_proc.
replicates	number of replicates used. Default is set to replicates=3

Value

Data.frame with standard deviation.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
sd<-sd_timepoint(df=a, replicates=3)
```

`select_indices` *Allows for selecting some peptide from input data*

Description

Function allows for picking indices from the inputs based on: peptide start or end residue, length, state or timepoint. If parameters set to NA, condition is skipped.

Usage

```
select_indices(df, start = NA, end = NA, length = NA, times = NA, states = NA)
```

Arguments

`df`	input file (output of output_tc or output_tp)
`start`	provide number for the staring residue, default NA
`end`	provide number for the end residue, default NA
`length`	provide max length of the peptide
`times`	timepoints, only for the output_tp functions
`states`	states, only for the output_tc functions

Value

Row indices of the peptides that are fulfilling the conditions required.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tp(file_nm)
indb<-select_indices(a,length=12, start=100, end=200)
smaller_df<-a[indb,]
```

significant_peptide_uptake

Function returns which peptides are significantly based of pv_cutoff and Critial interval

Description

Returns data frame with significant peptides.

Usage

```
significant_peptide_uptake(df_av, pv, sd, pv_cutoff = 0.01, replicates = 3)
```

Arguments

df_av	data.frame with averages created using ave_timepoint() function
pv	data.frame with pvalues created using pv_timepoint() function
sd	data.frame with standard deviations created using sd_timepoint() function
pv_cutoff	cuttoff for Critical interval. Default=0.01
replicates	number of replicates as default set to 3.

Value

ranges per set

summary_sd_CI

Provides summary table with Critical interval and standard deviation within the set.

Description

Returns summary data. Function returns: Protein states, timepoints, number of replicates, # peptides, % coveregae, average peptide length and redundancy.

Usage

```
summary_sd_CI(filepath, replicates = 3)
```

Arguments

filepath	filepath to the input file. Input file is All_results table from HDX_Examiner, where all the fields are marked for export.
replicates	number of replicates. Default set to 3.

Value

Returns summary table.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- summary_sd_CI(file_nm, replicates=3)
```

---

uptake_plots *Uptake plots*

Description

Uptake plots per peptide

Usage

```
uptake_plots(
  input_data,
  timepoints,
  replicates = 3,
  cola = NA,
  seq_match = TRUE
)
```

Arguments

input_data	output from function output_tp(..., percent=T)
timepoints	the labeling times
replicates	replicates
cola	colors, default NA
seq_match	Flag TRUE or FALSE, default TRUE, match sequence of the protein states

Value

Uptake plots

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tc(file_nm, percent=TRUE)
x=c(3,60, 1800, 72000)
uptake_plots(a, x)
```

verbose_timecourse_output

Returns csv with averages from analysis for procent deuteration file, standard deviation for time courses.

Description

Returns information from analysis and save it as csv file. Sets are compared to the first state in the input file.

Usage

```
verbose_timecourse_output(filepath, output_name, replicates = 3, ...)
```

Arguments

filepath	path to All.Data.csv input from HDX-Examiner.
output_name	name of the output in csv format.
replicates	number of replicates used
...	other variables for output_tc

Value

csv with analysis for procent deuteration: standard deviation, for all protein states for time courses.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
verbose_timecourse_output(file_nm,tempfile(), replicates=3)
names_states<- nm_states(file_nm)
verbose_timecourse_output(file_nm, tempfile(), seq_match=TRUE, percent=TRUE,
states=names_states, replicates=3, times="3.00s")
```

verbose_timepoint_output

Returns csv with averages from analysis for uptake file, standard deviation, p-values.

Description

Returns information from analysis and save it as csv file. Sets are compared to the first state in the input file.

Usage

```
verbose_timepoint_output(filepath, output_name, replicates = 3, ...)
```

Arguments

filepath	path to All.Data.csv input from HDX-Examiner.
output_name	name of the output in csv format.
replicates	number of replicates used
...	other variables for output_tp

Value

csv with analysis for uptake file, standard deviation, p-values for all protein states.

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
verbose_timepoint_output(file_nm, tempfile())
names_states<- nm_states(file_nm)
verbose_timepoint_output(file_nm, tempfile(), seq_match=TRUE, percent=TRUE,
states=names_states, replicates=3, times="3.00s")
```

---

vol_tp *Preparatory function for volcano plot*

Description

Returns volcano plots

Usage

```
vol_tp(df1, pv, CI, pv_cutoff = 0.01, cola)
```

Arguments

df1	differences in averages data.frame calculated using diff_ave function
pv	pvalues dataframes calculated using pv_timepoint function
CI	critical interval, here is multiple sets are using maximun CI is used.
pv_cutoff	p-value cutoff here set up to 0.01
cola	color pallette for different Protein States. As default Paired pallette from color.Brewer is used.

Value

volcano plots

`woods_CI_plot` *Returns a woods plot for comparisons of the timepoints samples*

Description

Modification of butterfly plot. x axis residues. y axis % deuteration for Peptides are compared between the sets for the significance change between sets. If there is significant change beteween sets peptides are plotted for all timepoints. Significanty different timepoints for the peptides are colored. Peptides ranges are plotted as a line at corresponding % deuteration values.

Usage

```
woods_CI_plot(
  thP,
  th,
  replicates = 3,
  pv_cutoff = 0.01,
  states,
  CI_factor = 1,
  ylim = c(0, 120),
  ...
)
```

Arguments

`thP`	output of output_tcourse_proc() function. Raw data for procent deuteration for time courses
`th`	output of output_tcourse() function. Raw data for uptake deuteration for time courses
`replicates`	number of replicates in sample. Default set to 3.
`pv_cutoff`	p-value cutoff here set up to 0.01
`states`	Protein states from the set. As default all states are chosen.
`CI_factor`	Multiplication factor for Critical Interval. Allows for more restrictive selection of Critial interval.
`ylim`	y axis limit
`...`	other variables

Value

Woods plots with chosen statistically different peptides

Examples

```
file_nm<-system.file("extdata", "All_results_table.csv", package = "HDXBoxeR")
a<- output_tc(file_nm)
b<-output_tc(file_nm, percent=TRUE)
woods_CI_plot(thP=b, th=a, pv_cutoff = 0.001, CI_factor = 1, replicates=3)
```

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