

Package: MSstatsShiny (via r-universe)

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Type Package

Title MSstats GUI for Statistical Analysis of Proteomics Experiments

Version 1.15.9

Description MSstatsShiny is an R-Shiny graphical user interface (GUI) integrated with the R packages MSstats, MSstatsTMT, and MSstatsPTM. It provides a point and click end-to-end analysis pipeline applicable to a wide variety of experimental designs. These include data-dependent acquisitions (DDA) which are label-free or tandem mass tag (TMT)-based, as well as DIA, SRM, and PRM acquisitions and those targeting post-translational modifications (PTMs). The application automatically saves users selections and builds an R script that recreates their analysis, supporting reproducible data analysis.

License Artistic-2.0

Depends R (>= 4.2)

Imports shiny (>= 1.5.0), shinyBS, shinyjs, shinybusy, dplyr, ggplot2, plotly, data.table, Hmisc, shinyFiles, MSstats, MSstatsBig, MSstatsTMT, MSstatsPTM, MSstatsConvert, gplots, marray, DT, readxl, ggrepel, uuid, utils, stats, htmltools, methods, tidyr, grDevices, graphics, mockery, MSstatsBioNet, shinydashboard, arrow, tools, MSstatsResponse, stringr, http

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<i>annotation.mine</i>	<i>Example annotation file for Spectromine</i>
------------------------	--

Description

data.frame mapping Spectromine run names to the corresponding bioreplicates and conditions. Used as input to preprocessing function, converting data into MSstats format.

Format

data.frame

Examples

```
data(annotation.mine)
head(annotation.mine)
```

<i>annotation.mq</i>	<i>Example annotation file for MaxQuant</i>
----------------------	---

Description

data.frame mapping MaxQuant run names to the corresponding bioreplicates and conditions. Used as input to preprocessing function, converting data into MSstats format.

Format

data.frame

Examples

```
data(annotation.mq)
head(annotation.mq)
```

`annotation.pd`*Example annotation file for PD*

Description

data.frame mapping PD run names to the corresponding bioreplicates and conditions. Used as input to preprocessing function, converting data into MSstats format.

Format

data.frame

Examples

```
data(annotation.pd)
head(annotation.pd)
```

`apply_adj`*Main PTM adjustment function*

Description

Main PTM function to model MSstatsShiny data.

Usage

```
apply_adj(ptm_model, protein_model)
```

Arguments

`ptm_model` output of MSstats modeling function modeling PTMs
`protein_model` output of MSstats modeling function modeling unmodified proteins

Value

list of PTM modeling results

Examples

```
model = MSstatsPTM::groupComparisonPTM(MSstatsPTM::summary.data)
apply_adj(model$PTM.Model, model$PROTEIN.Model)
```

dia_skyline_model	<i>Example of Skyline DDA dataset modeled using MSstats groupComparison function.</i>
-------------------	---

Description

Data includes one list with two data.tables named ComparisonResult and ModelQC and another list of model details named FittedModel. ComparisonResult shows an overview of all proteins modeled in the system. ModelQC provides a report on the quality control checks of each protein in the dataset.

Format

list

Examples

```
data(dia_skyline_model)
head(dia_skyline_model)
```

dia_skyline_summarized	<i>Example of Skyline DDA dataset processed using MSstats summarization function.</i>
------------------------	---

Description

Data includes one list with two data.tables named FeatureLevelData and ProteinLevelData and a string value SummaryMethod. FeatureLevelData shows the unsummarized feature level data. ProteinLevelData shows the data summarized up to the protein level and is used for modeling the data.

Format

list

Examples

```
data(dia_skyline_summarized)
head(dia_skyline_summarized)
```

evidence	<i>Example evidence file for MaxQuant</i>
----------	---

Description

data.frame containing output of MaxQuant. Used in examples.

Format

data.frame

Examples

```
data(evidence)
head(evidence)
```

example_dia_skyline	<i>Example of input Skyline DDA dataset.</i>
---------------------	--

Description

Used as input data to MSstats workflow. Data includes one data.table which is the output of Skyline.

Format

data.frame

Details

The raw data (input data for MSstats) is required to contain variable of ProteinName, PeptideSequence, PrecursorCharge, FragmentIon, ProductCharge, IsotopeLabelType, Condition, BioReplicate, Run, Intensity. The variable names should be fixed. If the information of one or more columns is not available for the original raw data, please retain the column variables and type in fixed value. For example, the original raw data does not contain the information of PrecursorCharge and ProductCharge, we retain the column PrecursorCharge and ProductCharge and then type in NA for all transitions in RawData. Variable Intensity is required to be original signal without any log transformation and can be specified as the peak of height or the peak of area under curve.

Examples

```
data(example_dia_skyline)
head(example_dia_skyline)
```

`example_skyline_annotation`*Example annotation file*

Description

data.frame mapping Skyline run names to the corresponding bioreplicates and conditions. Used as input to preprocessing function, converting data into MSstats format.

Format

data.frame

Examples

```
data(example_skyline_annotation)
head(example_skyline_annotation)
```

`expdesServer`*Expdes Server module for future experiments*

Description

Expdes Server module for future experiments

Usage

```
expdesServer(
  input,
  output,
  session,
  parent_session,
  loadpage_input,
  qc_input,
  app_template = reactive(TEMPLATES$default),
  data_comparison,
  preprocess_data = NULL,
  statmodel_contrast = NULL
)
```

Arguments

input	input object to capture different ui element values
output	to render and create elements
session	session current module
parent_session	session of the main calling module
loadpage_input	input object from loadpage UI
qc_input	input object from QC UI
app_template	reactive returning the selected template name
data_comparison	function for group comparisons
preprocess_data	function returning preprocessed data
statmodel_contrast	reactiveValues object containing the contrast matrix from statmodel

Value

list object with user selected options and matrix build

Examples

NA

expdesUI

Expdes UI module for future experiments UI.

Description

This function sets up the Expdes UI where it consists of several, options for users to select and generate plots.

Usage

```
expdesUI(id)
```

Arguments

id	namespace prefix for the module
----	---------------------------------

Value

This function returns nothing, as it sets up the Expdes UI

Examples

NA

groupComparisonPlots2 *Plotting functionality for QC plots*

Description

General plotting code to produce all QC plots in the application

Usage

```
groupComparisonPlots2(  
  data = data,  
  type = type,  
  sig = 0.05,  
  FCcutoff = FALSE,  
  logBase.pvalue = 10,  
  ylimUp = FALSE,  
  ylimDown = FALSE,  
  xlimUp = FALSE,  
  x.axis.size = 10,  
  y.axis.size = 10,  
  dot.size = 3,  
  text.size = 4,  
  legend.size = 13,  
  ProteinName = TRUE,  
  colorkey = TRUE,  
  numProtein = 100,  
  clustering = "both",  
  width = 10,  
  height = 10,  
  which.Comparison = "all",  
  which.Protein = "all",  
  address = "",  
  savePDF = FALSE  
)
```

Arguments

data	'ComparisonResult' in testing output from function groupComparison.
type	choice of visualization. "VolcanoPlot" represents volcano plot of log fold changes and adjusted p-values for each comparison separately. "Heatmap" represents heatmap of adjusted p-values for multiple comparisons. "ComparisonPlot" represents comparison plot of log fold changes for multiple comparisons per protein.
sig	FDR cutoff for the adjusted p-values in heatmap and volcano plot. level of significance for comparison plot. 100(1-sig)% confidence interval will be drawn. sig=0.05 is default.

FCcutoff	for volcano plot or heatmap, whether involve fold change cutoff or not. FALSE (default) means no fold change cutoff is applied for significance analysis. FC-cutoff = specific value means specific fold change cutoff is applied.
logBase.pvalue	for volcano plot or heatmap, (-) logarithm transformation of adjusted p-value with base 2 or 10(default).
ylimUp	for all three plots, upper limit for y-axis. FALSE (default) for volcano plot/heatmap use maximum of -log2 (adjusted p-value) or -log10 (adjusted p-value). FALSE (default) for comparison plot uses maximum of log-fold change + CI.
ylimDown	for all three plots, lower limit for y-axis. FALSE (default) for volcano plot/heatmap use minimum of -log2 (adjusted p-value) or -log10 (adjusted p-value). FALSE (default) for comparison plot uses minimum of log-fold change - CI.
xlimUp	for Volcano plot, the limit for x-axis. FALSE (default) for use maximum for absolute value of log-fold change or 3 as default if maximum for absolute value of log-fold change is less than 3.
x.axis.size	size of axes labels, e.g. name of the comparisons in heatmap, and in comparison plot. Default is 10.
y.axis.size	size of axes labels, e.g. name of targeted proteins in heatmap. Default is 10.
dot.size	size of dots in volcano plot and comparison plot. Default is 3.
text.size	size of ProteinName label in the graph for Volcano Plot. Default is 4.
legend.size	size of legend for color at the bottom of volcano plot. Default is 7.
ProteinName	for volcano plot only, whether display protein names or not. TRUE (default) means protein names, which are significant, are displayed next to the points. FALSE means no protein names are displayed.
colorkey	TRUE(default) shows colorkey.
numProtein	The number of proteins which will be presented in each heatmap. Default is 100. Maximum possible number of protein for one heatmap is 180.
clustering	Determines how to order proteins and comparisons. Hierarchical cluster analysis with Ward method(minimum variance) is performed. 'protein' means that protein dendrogram is computed and reordered based on protein means (the order of row is changed). 'comparison' means comparison dendrogram is computed and reordered based on comparison means (the order of comparison is changed). 'both' means to reorder both protein and comparison. Default is 'protein'.
width	width of the saved file. Default is 10.
height	height of the saved file. Default is 10.
which.Comparison	list of comparisons to draw plots. List can be labels of comparisons or order numbers of comparisons from levels(data\$Label), such as levels(testResultMultiComparisons\$Comparison). Default is "all", which generates all plots for each protein.
which.Protein	Protein list to draw comparison plots. List can be names of Proteins or order numbers of Proteins from levels(testResultMultiComparisons\$ComparisonResult\$Protein). Default is "all", which generates all comparison plots for each protein.

address	the name of folder that will store the results. Default folder is the current working directory. The other assigned folder has to be existed under the current working directory. An output pdf file is automatically created with the default name of "VolcanoPlot.pdf" or "Heatmap.pdf" or "ComparisonPlot.pdf". The command address can help to specify where to store the file as well as how to modify the beginning of the file name. If address=FALSE, plot will be not saved as pdf file but showed in window.
savePDF	Boolean input passed from user on whether or not to save the plot to a PDF.

Value

PDF or console plot

Examples

```
data("dia_skyline_model")
groupComparisonPlots2(dia_skyline_model$ComparisonResult, type="VolcanoPlot",
                      address=FALSE)
```

helpUI

Help UI module for help page.

Description

This module shows the help page for general documentation

Usage

```
helpUI(id)
```

Arguments

id	namespace prefix for the module
----	---------------------------------

Value

This function returns nothing, as it sets up the Help UI

Examples

```
NA
```

`homeUI`*Home UI module for home page.*

Description

This function generates the home user interface for MSstatsShiny, a web tool for the statistical analysis of quantitative proteomic data built around the R packages MSstats, MSstatsTMT, and MSstatsPTM.

Usage

```
homeUI(id)
```

Arguments

`id` namespace prefix for the module

Value

This function returns nothing, as it sets up the Home UI

Examples

```
NA
```

`launch_MSstatsShiny`*Run MSstatsShiny Application*

Description

Main function to run MSstatsShiny. All other functions in this package are run automatically.

Usage

```
launch_MSstatsShiny(  
  launch_app = TRUE,  
  port = getOption("shiny.port"),  
  host = getOption("shiny.host", "127.0.0.1"),  
  testMode = FALSE  
)
```

Arguments

launch_app	One of TRUE or FALSE indicating whether or not to run application. Default is TRUE.
port	(optional) Specify port the application should list to.
host	(optional) The IPv4 address that the application should listen on.
testMode	One of TRUE or FALSE indicating whether or not to run the application in test mode. Default is FALSE.

Value

Running Shiny Application

Examples

```
## Not run:
## To run app set launch_app=TRUE
launch_MSstatsShiny(launch_app=FALSE, testMode=FALSE)

## End(Not run)
```

lf_model

Main LF modeling function for MSstatsShiny application

Description

Main LF function to model MSstatsShiny data.

Usage

```
lf_model(data, contrast.matrix, busy_indicator = TRUE)
```

Arguments

data	summarized data from output of MSstats summarization function.
contrast.matrix	contrast matrix specifying which conditions should be compared
busy_indicator	Boolean indicator indicating whether or not to display shiny waiting indicator.

Value

list of LF modeling results

Examples

```
data("dia_skyline_summarized")
comparison <- matrix(c(1, -1, 0, 0, 0, 0, 0, 0, 0), nrow=1)
row.names(comparison) = "1 vs 128"
colnames(comparison) = c("1", "128", "16", "2", "256",
                        "32", "4", "512", "64", "8")
model_lf_test = lf_model(dia_skyline_summarized, comparison,
                        busy_indicator = FALSE)
```

`lf_summarization_loop` *Main LF calculation summarization function for MSstatsShiny application*

Description

Main LF function to calculate MSstatsShiny results.

Usage

```
lf_summarization_loop(data, qc_input, loadpage_input, busy_indicator = TRUE)
```

Arguments

`data` Data converted into MSstats format.

`qc_input` options for data processing input by the user from data processing page.

`loadpage_input` options for data processing input by the user from data upload page.

`busy_indicator` Boolean indicator indicating whether or not to display shiny waiting indicator.

Value

list of LF Summarization results

Examples

```
data("example_dia_skyline")
data("example_skyline_annotation")
testdata = MSstats::SkylinetoMSstatsFormat(example_dia_skyline,
                                           annotation = example_skyline_annotation,
                                           filter_with_Qvalue = TRUE,
                                           qvalue_cutoff = 0.01,
                                           fewMeasurements="remove",
                                           removeProtein_with1Feature = TRUE,
                                           use_log_file = FALSE)

## Source app functionality
qc_input = list()
```

```

loadpage_input = list()
qc_input$norm = "equalizeMedians"
qc_input$log = 2
qc_input$names = NULL
qc_input$features_used = "all"
code_n_feat=3
qc_input$censInt = "NA"
qc_input$MBi = TRUE
qc_input$remove50 = FALSE
qc_input$maxQC = 0.999
qc_input$null = FALSE
qc_input$null1 = FALSE
qc_input$summaryMethod = "TMP"
loadpage_input$DDA_DIA = "LF"
lf_summarization_loop(testdata, qc_input,loadpage_input, busy_indicator=FALSE)

```

loadpageServer

Loadpage Server module for data selection and upload server.

Description

This function sets up the loadpage server where it consists of several options for users to select and upload files. After the Phase 2 split, the orchestrator below keeps only:

Usage

```
loadpageServer(id, parent_session, is_web_server = FALSE, app_template = NULL)
```

Arguments

id	namespace prefix for the module
parent_session	session of the main calling module
is_web_server	boolean indicating if the app is running on a web server
app_template	reactive (or NULL) returning the selected template

Details

- the module signature and condition_metadata reactiveVal,
- the shinyFiles browser block (it produces the local_big_file_path / local_big_diann_path reactives that the proceed-validation helper consumes, so it must remain co-located with the module's reactive scope),
- the six helper registrations in order (register_loadpage_preview, register_loadpage_visibility_observers, register_loadpage_converter_ui, register_loadpage_proceed_validation, register_loadpage_data_load, register_loadpage_summary),
- the final public return(list(input, getData, getConditionMetadata)).

Each helper lives in its own file (R/loadpage-server-*.R); see those files for the moved code blocks.

Value

input object with user selected options

Examples

NA

loadpageUI	<i>Loadpage UI module for data selection and upload UI.</i>
------------	---

Description

This function sets up the loadpage UI where it consists of several options for users to select and upload files.

Usage

loadpageUI(id)

Arguments

id namespace prefix for the module

Value

This function returns nothing, as it sets up the loadpage UI

Examples

NA

msstatsHelpUI	<i>Help MSSStats UI module for msstats help page.</i>
---------------	---

Description

This module shows the msstats help page for general documentation

Usage

msstatsHelpUI(id)

Arguments

id namespace prefix for the module

Value

This function returns nothing, as it sets up the MSStats Help UI

Examples

NA

msstatsTmtHelpUI	<i>Help MSStats UI module for msstatstmt help page.</i>
------------------	---

Description

This module shows the msstats help page for general documentation

Usage

```
msstatsTmtHelpUI(id)
```

Arguments

id	namespace prefix for the module
----	---------------------------------

Value

This function returns nothing, as it sets up the MSStatstmts Help UI

Examples

NA

networkUI	<i>Network UI module for visualizing protein regulatory networks from INDRA.</i>
-----------	--

Description

Network UI module for visualizing protein regulatory networks from INDRA.

Usage

```
networkUI(id)
```

Arguments

id	namespace prefix for the module
----	---------------------------------

proteinGroups	<i>Example ProteinGroups file for MaxQuant</i>
---------------	--

Description

data.frame containing output of ProteinGroups MaxQuant file. Used in examples.

Format

data.frame

Examples

```
data(proteinGroups)
head(proteinGroups)
```

QC_check	<i>Quick QC value check</i>
----------	-----------------------------

Description

Quick QC value check for LF vs TMT

Usage

```
QC_check(qc_input, loadpage_input)
```

Arguments

- qc_input options for data processing input by the user from data processing page.
- loadpage_input options for data processing input by the user from data upload page.

Value

string

Examples

```
qc_input = list(null=TRUE)
loadpage_input = list(null=TRUE)
QC_check(qc_input,loadpage_input)
```

qcServer

QC Server module for data processing

Description

This function sets up the QC server to process data based on user selected inputs

Usage

```
qcServer(
  input,
  output,
  session,
  parent_session,
  loadpage_input,
  get_data,
  app_template = NULL,
  get_condition_metadata = NULL
)
```

Arguments

input	input object to capture different ui element values
output	to render and create elements
session	session current module
parent_session	session of the main calling module
loadpage_input	input object from loadpage UI
get_data	stored function that returns the data from loadpage
app_template	reactive (or NULL) returning the selected template name (e.g. TEMPLATES\$default)
get_condition_metadata	reactive (or NULL) returning the condition metadata table

Value

a list with four elements: input (the module's input object), preprocessData (reactive returning the preprocessed data), turnoverRatios (reactive returning the turnover ratios, or the uploaded ratios when those override them), and tracerConstants (reactive returning the tracer-constant provenance record snapshotted at Run)

Examples

```
NA
```

`qcUI`*QC UI module for data processing UI.*

Description

This function sets up the QC UI where it consists of several, options for users to process data based on previously selected fragments.

Usage

```
qcUI(id)
```

Arguments

<code>id</code>	namespace prefix for the module
-----------------	---------------------------------

Value

This function returns nothing, as it sets up the QC UI

Examples

```
NA
```

`radioTooltip`*Custom function to create radio tool tips*

Description

Used in UI files to create HTML vizualizations

Usage

```
radioTooltip(  
  id,  
  choice,  
  title,  
  placement = "bottom",  
  trigger = "hover",  
  options = NULL  
)
```

Arguments

id	input id
choice	user selection
title	title of object
placement	where should tooltip be shown
trigger	how should prompt be shown
options	additional options to pass to function

Value

HTML object

Examples

```
radioTooltip("testid", "test_choice", "test_title")
```

raw.mine

Example output file Spectromine

Description

data.frame containing output of Spectromine. Used in examples.

Format

data.frame

Examples

```
data(raw.mine)
head(raw.mine)
```

`raw.om`*Example output file Spectromine*

Description

data.frame containing output of Spectromine. Used in examples.

Format

data.frame

Examples

```
data(raw.om)
head(raw.om)
```

`raw.pd`*Example output file PD*

Description

data.frame containing output of PD. Used in examples.

Format

data.frame

Examples

```
data(raw.pd)
head(raw.pd)
```

server	<i>Server function for the MSstatsShiny app</i>
--------	---

Description

This functions generates the Server object for MSstatsShiny app.

Usage

```
server(input, output, session)
```

Arguments

input	shiny server input
output	shiny server output
session	session object for shiny to connect to

Value

Server object for shinyUI

Examples

```
NA
```

statmodelServer	<i>Statmodel Server module for stat inference</i>
-----------------	---

Description

This function sets up the Statmodel server to process data based on user selected inputs

Usage

```
statmodelServer(
  id,
  parent_session,
  loadpage_input,
  qc_input,
  get_data,
  preprocess_data,
  app_template = reactive(TEMPLATES$default),
  turnover_ratios = reactive(NULL),
  condition_metadata = reactive(NULL),
  tracer_constants = reactive(NULL)
)
```

Arguments

id	namespace prefix for the module
parent_session	session of the main calling module
loadpage_input	input object from loadpage UI
qc_input	input object from QC UI
get_data	stored function that returns the data from loadpage
preprocess_data	stored function that returns preprocessed data
app_template	reactive returning the selected template name (e.g. TEMPLATES\$default)
turnover_ratios	reactive returning the calculated turnover ratios
condition_metadata	reactive returning the condition metadata table
tracer_constants	reactive returning the tracer-constant provenance record snapshotted by the QC page at Run (values / source / file), or NULL when the data-processing page has not been run in this session

Value

list object with user selected options and matrix build

Examples

NA

statmodelUI	<i>Statmodel UI module for statistical inference UI.</i>
-------------	--

Description

This function sets up the Statmodel UI where it consists of several, options for users to select and upload files.

Usage

statmodelUI(id)

Arguments

id	namespace prefix for the module
----	---------------------------------

Value

This function returns nothing, as it sets up the Statmodel UI

Examples

NA

tmt_model

Main TMT modeling function for MSstatsShiny application

Description

Main TMT function to model MSstatsShiny data.

Usage

```
tmt_model(data, input, contrast.matrix, busy_indicator = TRUE)
```

Arguments

data summarized data from output of MSstats summarization function.
input options for data processing input by the user
contrast.matrix contrast matrix specifying which conditions should be compared
busy_indicator Boolean indicator indicating whether or not to display shiny waiting indicator.

Value

list of TMT modeling results

Examples

```
raw.pd = data.table::fread(system.file("tinytest/raw_data/PDTMT/pdmtmt_input.csv",
                                     package = "MSstatsConvert"))
annotation.pd = data.table::fread(system.file("tinytest/raw_data/PDTMT/pd_annotation.csv",
                                             package = "MSstatsConvert"))

testdata <- MSstatsTMT::PDtoMSstatsTMTFormat(raw.pd,
                                             annotation.pd,
                                             use_log_file = FALSE
                                             )#'

qc_input = list()
loadpage_input = list()
qc_input$summarization = "msstats"
qc_input$norm = "equalizeMedians"
qc_input$log = 2
qc_input$names = NULL
qc_input$features_used = "all"
code_n_feat=3
qc_input$censInt = "NA"
```

```

qc_input$MBi = TRUE
qc_input$remove50 = FALSE
qc_input$maxQC = 0.999
qc_input$null = FALSE
qc_input$null1 = FALSE
loadpage_input$DDA_DIA = "LF"
qc_input$global_norm = TRUE
qc_input$reference_norm = TRUE
qc_input$remove_norm_channel = TRUE
qc_input$maxQC1 = NULL
qc_input$moderated = FALSE
qc_input$summaryMethod = "TMP"
summarization_tmt_test = tmt_summarization_loop(testdata, qc_input, loadpage_input,
                                                busy_indicator = FALSE)

comparison=matrix(c(-1,0,0,1),nrow=1)
row.names(comparison) = "1-0.125"
colnames(comparison) = c("0.125", "0.5", "0.667", "1")

model_tmt_test = tmt_model(summarization_tmt_test, qc_input, comparison,
                           busy_indicator = FALSE)

```

tmt_pd_model	<i>Example of TMT dataset modeled using MSstatsTMT groupComparisonTMT function.</i>
--------------	---

Description

Data includes one list with two data.tables named ComparisonResult and ModelQC and another list of model details named FittedModel. ComparisonResult shows an overview of all proteins modeled in the system. ModelQC provides a report on the quality control checks of each protein in the dataset.

Format

list

Examples

```

data(tmt_pd_model)
head(tmt_pd_model)

```

tmt_pd_summarized	<i>Example of TMT dataset processed using MSstatsTMT summarization function.</i>
-------------------	--

Description

Data includes one list with two data.tables named FeatureLevelData and ProteinLevelData. FeatureLevelData shows the unsummarized feature level data. ProteinLevelData shows the data summarized up to the protein level and is used for modeling the data.

Format

list

Examples

```
data(tmt_pd_summarized)
head(tmt_pd_summarized)
```

tmt_summarization_loop	<i>Main TMT summarization calculation function for MSstatsShiny application</i>
------------------------	---

Description

Main TMT function to calculate MSstatsShiny results.

Usage

```
tmt_summarization_loop(data, qc_input, loadpage_input, busy_indicator = TRUE)
```

Arguments

data	Data converted into MSstats format.
qc_input	options for data processing input by the user from data processing page.
loadpage_input	options for data processing input by the user from data upload page.
busy_indicator	Boolean indicator indicating whether or not to display shiny waiting indicator.

Value

list of TMT summarization results

Examples

```

raw.pd = data.table::fread(system.file("tinytest/raw_data/PDTMT/pdmtmt_input.csv",
                                       package = "MSstatsConvert"))
annotation.pd = data.table::fread(system.file("tinytest/raw_data/PDTMT/pd_annotation.csv",
                                              package = "MSstatsConvert"))

testdata <- MSstatsTMT::PDtoMSstatsTMTFormat(raw.pd,
                                             annotation.pd,
                                             use_log_file = FALSE
                                             )

qc_input = list()
loadpage_input = list()
qc_input$summarization = "msstats"
qc_input$norm = "equalizeMedians"
qc_input$log = 2
qc_input$names = NULL
qc_input$features_used = "all"
code_n_feat=3
qc_input$censInt = "NA"
qc_input$MBi = TRUE
qc_input$remove50 = FALSE
qc_input$maxQC = 0.999
qc_input$null = FALSE
qc_input$null1 = FALSE
loadpage_input$DDA_DIA = "LF"
qc_input$global_norm = TRUE
qc_input$reference_norm = TRUE
qc_input$remove_norm_channel = TRUE
qc_input$maxQC1 = NULL
qc_input$summaryMethod = "TMP"
summarization_tmt_test = tmt_summarization_loop(testdata, qc_input,loadpage_input,
                                                busy_indicator = FALSE)

```

uiObject

UI function for the MSstatsShiny app

Description

This functions generates the UI object for MSstatsShiny app. Responsible for generating 5 nav pages homepage, data upload page, data processing page, statistical inference and future experiments.

Usage

```
uiObject()
```

Value

UI object for shinyUI

Examples

NA

visualizeNetworkServer

Server logic for network visualization module

Description

Server logic for network visualization module

Usage

```
visualizeNetworkServer(  
  id,  
  parent_session,  
  dataComparison,  
  app_template = reactive(TEMPLATES$default)  
)
```

Arguments

id	Module ID string
parent_session	Parent Shiny session
dataComparison	Reactive expression containing comparison data
app_template	Reactive returning the selected template name (e.g. TEMPLATES\$default)

Value

None (side effects only)

xy_str	<i>Simple function to return coordinates</i>
--------	--

Description

Used in experimental design to create vizualization

Usage

```
xy_str(e)
```

Arguments

e	input function provided by user
---	---------------------------------

Value

Character with x and y coordinates

Examples

```
xy_str(list(x=5.0,y=2.0))
```

zip_and_copy_plot	<i>Zip PDF files and copy to download destination</i>
-------------------	---

Description

Zip PDF files and copy to download destination

Usage

```
zip_and_copy_plot(pdf_files, dest_file)
```

Arguments

pdf_files	character vector of PDF file paths
dest_file	destination file path for the download

Value

TRUE if successful, FALSE otherwise

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