Package ‘MSstatsShiny’

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Type Package
Title MSstats GUI for Statistical Analysis of Proteomics Experiments
Version 1.6.0
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
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Suggests rmarkdown, tinytest, sessioninfo, knitr, testthat (>= 3.0.0), shinytest2,
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**annotation.mine**  
*Example annotation file for Spectromine*

---

**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 )

---

**annotation.mq**  
*Example annotation file for MaxQuant*

---

**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**

```r
model = MSstatsPTM::groupComparisonPTM(MSstatsPTM::summary.data, data.type = "LabelFree")
apply_adj(model$PTM.Model, model$PROTEIN.Model)
```
**dia_skyline_model**  
*Example of Skyline DDA dataset modeled using MSstats groupComparison function.*

**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**

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

---

**dia_skyline_summarized**  
*Example of Skyline DDA dataset processed using MSstats summarization function.*

**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**

```r
data(dia_skyline_summarized)  
head(dia_skyline_summarized)
```
**evidence**  
*Example evidence file for MaxQuant*

**Description**  
Data.frame containing output of MaxQuant. Used in examples.

**Format**  
data.frame

**Examples**
```r
data(evidence)  
head(evidence)
```

---

**example_dia_skyline**  
*Example of input Skyline DDA dataset.*

**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**
```r
data(example_dia_skyline)  
head(example_dia_skyline)
```
**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**

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

**Usage**

expdesServer(
  input, output, session, parent_session, loadpage_input, qc_input, statmodel_input, data_comparison
)

**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
statmodel_input input object from Statmodel UI
data_comparison function for group comparisons

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

```r


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$Label), such as levels(testResultMultiComparisons$ComparisonResult$Label). 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.
helpUI

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
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
)
**lf_model**

**Description**

Main LF function to model MSstatsShiny data.

**Usage**

```r
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

```r
data("dia_skyline_summarized")
comparison <- matrix(c(1, -1, 0, 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)
```

Description

Main LF calculation summarization function for MSstatsShiny application.

Usage

```r
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

```r
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

```r
qc_input = list()
```
loadpage_server

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
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.

Usage

loadpageServer(id, parent_session)

Arguments

id namespace prefix for the module
parent_session session of the main calling module

Value

input object with user selected options

Examples

NA
loadpageUI

Loadpage UI module for data selection and upload UI.

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

Help MSStats UI module for msstats help page.

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
MSstatsShiny: An R-shiny based package for detecting differentially abundant proteins, integrated with the MSstats family of packages.

Description
A set of tools for detecting differentially abundant proteins in shotgun mass spectrometry-based proteomic experiments. The package can handle a variety of acquisition types, including label free, DDA, DIA, and TMT. The package includes tools to convert raw data from different spectral processing tools, summarize feature intensities, and fit a linear mixed effects model. The GUI supports different biological queries including those targeting the global proteome and post translational modifications. Additionally the package includes functionality to plot a variety of data visualizations.

functions
- `launch_MSstatsShiny`: Main function to launch the application.
- `groupComparisonPlots2`: Generates MSstatsShiny plots.
- `lf_summarization_loop`: Summarization for LF experiments.
- `tmt_summarization_loop`: Summarization for TMT experiments.
- `lf_model`: Modeling for LF experiments.
- `tmt_model`: Modeling for TMT experiments.

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See Also
Useful links:
- Report bugs at https://github.com/Vitek-Lab/MSstatsShiny/issues
### msstatsTmtHelpUI

*Help MSStats UI module for msstatsmt help page.*

**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

---

### proteinGroups

*Example ProteinGroups file for MaxQuant*

**Description**

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

**Format**

`data.frame`

**Examples**

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

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

Value
input object with user selected options

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
id: namespace prefix for the module
**Value**

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

**Examples**

NA

**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)
```
### radioTooltip

**Custom function to create radio tool tips**

**Description**

Used in UI files to create HTML visualizations

**Usage**

```r
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**

```r
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

Server function for the MSstatsShiny app

Description

This function generates the Server object for MSstatsShiny app.

Usage

```r
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

Statmodel Server module for stat inference

Description

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

Usage

```r
statmodelServer(
  input,
  output,
  session,
  parent_session,
  loadpage_input,
  qc_input,
  get_data,
  preprocess_data
)
```
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
- **get_data**: stored function that returns the data from loadpage
- **preprocess_data**: stored function that returns preprocessed data

Value

- list object with user selected options and matrix build

Examples

NA

---

**statmodelUI**

*Statmodel UI module for statistical inference UI.*

Description

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

Usage

```r
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

```r
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

```r
data(raw.pd, package = "MSstatsTMT")
data(annotation.pd, package = "MSstatsTMT")

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

```r
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

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_summarization_loop

Format

list

Examples

data(tmt_pd_summarized)
head(tmt_pd_summarized)

tmt_summarization_loop

Main TMT summarization calculation function for MSstatsShiny application

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

data(raw.pd, package = "MSstatsTMT")
data(annotation.pd, package = "MSstatsTMT")

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
uiObject

Description

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

Usage

uiObject()

Value

UI object for shinyUI

Examples

NA
**xy_str**

---

**xy_str**  
*Simple function to return coordinates*

---

**Description**

Used in experimental design to create visualization

**Usage**

\[ xy_{str}(e) \]

**Arguments**

- \( e \)  
  input function provided by user

**Value**

Character with x and y coordinates

**Examples**

\[ xy_{str}(\text{list}(x=5.0, y=2.0)) \]
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