

# Package ‘MSstatsShiny’

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**Type** Package

**Title** MSstats GUI for Statistical Analysis of Proteomics Experiments

**Version** 1.12.0

**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

**Depends** R (>= 4.2)

**Imports** shiny, shinyBS, shinyjs, shinybusy, dplyr, ggplot2, plotly, data.table, Hmisc, MSstats, MSstatsTMT, MSstatsPTM, MSstatsConvert, gplots, marray, DT, readxl, ggrepel, uuid, utils, stats, htmltools, methods, tidyr, grDevices, graphics, mockery, MSstatsBioNet, shinydashboard, arrow, tools, MSstatsResponse

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---

|                              |                                                |
|------------------------------|------------------------------------------------|
| <code>annotation.mine</code> | <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)
```

---

|                            |                                             |
|----------------------------|---------------------------------------------|
| <code>annotation.mq</code> | <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 | <i>Example annotation file for PD</i> |
|---------------|---------------------------------------|

---

**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 | <i>Main PTM adjustment function</i> |
|-----------|-------------------------------------|

---

**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,
                                         data.type = "LabelFree")
apply_adj(model$PTM.Model, model$PROTEIN.Model)
```

---

|                   |                                                                                       |
|-------------------|---------------------------------------------------------------------------------------|
| dia_skyline_model | <i>Example of Sklyine 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 Sklyine 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`*Example evidence file for MaxQuant*

---

**Description**

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

**Format**

data.frame

**Examples**

```
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**

```
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

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
```

---

```
generateCytoscapeJSForShiny
```

---

*Generate Cytoscape JavaScript with Shiny event handling*

---

**Description**

This function wraps the package's `generateCytoscapeConfig()` function and adds Shiny-specific event handling for table highlighting

**Usage**

```
generateCytoscapeJSForShiny(
  node_elements,
  edge_elements,
  display_label_type = "id",
  container_id = "network-cy",
  module_id = "network"
)
```

**Arguments**

node\_elements    Node elements from package  
 edge\_elements    Edge elements from package  
 display\_label\_type    Column to display the label from the node table  
 container\_id    Network Visualization Container ID (default: 'network-cy')  
 module\_id    Module ID for Shiny Application (default: 'network')

**Value**

JavaScript code string with Shiny event handlers

---

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 | <i>Help UI module for help page.</i> |
|--------|--------------------------------------|

---

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 | <i>Home UI module for home page.</i> |
|--------|--------------------------------------|

---

**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 | <i>Run MSstatsShiny Application</i> |
|---------------------|-------------------------------------|

---

**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, 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.

**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 | <i>Help MSStats 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
```

---

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

---

### 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 msstatstmt 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

---

|           |                                                                                  |
|-----------|----------------------------------------------------------------------------------|
| 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)
```

---

|          |                                             |
|----------|---------------------------------------------|
| qcServer | <i>QC Server module for data processing</i> |
|----------|---------------------------------------------|

---

**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

---

|          |                             |
|----------|-----------------------------|
| 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)
```

---

|              |                                                  |
|--------------|--------------------------------------------------|
| radioTooltip | <i>Custom function to create radio tool tips</i> |
|--------------|--------------------------------------------------|

---

**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 | <i>Example output file Spectromine</i> |
|----------|----------------------------------------|

---

**Description**

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

**Format**

data.frame

**Examples**

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

---

|        |                                        |
|--------|----------------------------------------|
| raw.om | <i>Example output file Spectromine</i> |
|--------|----------------------------------------|

---

**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 functions generates the Server object for MSstatsShiny app.

**Usage**

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

**Arguments**

|                      |                                        |
|----------------------|----------------------------------------|
| <code>input</code>   | shiny server input                     |
| <code>output</code>  | shiny server output                    |
| <code>session</code> | 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
)
```

### 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      |

### 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 | <i>Main TMT modeling function for MSstatsShiny application</i> |
|-----------|----------------------------------------------------------------|

---

**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**

```
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$log = 2
qc_input$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**

```

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$log = 2
qc_input$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(input, output, session, parent_session, dataComparison)
```

### Arguments

|                |                                                |
|----------------|------------------------------------------------|
| input          | Shiny input object                             |
| output         | Shiny output object                            |
| session        | Shiny session object                           |
| parent_session | Parent Shiny session                           |
| dataComparison | Reactive expression containing comparison data |

### Value

None (side effects only)

---

xy\_str

*Simple function to return coordinates*


---

### 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))
```

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