

Package ‘omXplore’

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Type Package

Title Vizualization tools for 'omics' datasets with R

Version 1.2.3

Description This package contains a collection of functions (written as shiny modules) for the visualisation and the statistical analysis of omics data. These plots can be displayed individually or embedded in a global Shiny module.

Additionally, it is possible to integrate third party modules to the main interface of the package omXplore.

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Depends R (>= 4.5.0), methods

Imports DT, shiny, MSnbase, PSMATCH, SummarizedExperiment, MultiAssayExperiment, shinyBS, shinyjs, shinyjqui, RColorBrewer, gplots, highcharter, visNetwork, tibble, grDevices, stats, utils, htmlwidgets, vioplot, graphics, FactoMineR, dendextend, dplyr, factoextra, tidyr, nipals

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biocViews Software, ShinyApps, MassSpectrometry, DataRepresentation, GUI, QualityControl

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accessors	<i>Accessors functions</i>
-----------	----------------------------

Description

Functions used to access the additional plots in the instances of the class MultiAssayExperiment.

Usage

```
get_adjacencyMatrix(object, ...)

## S4 method for signature 'SummarizedExperiment'
get_adjacencyMatrix(object)

get_design(object, ...)

## S4 method for signature 'MultiAssayExperiment'
get_design(object)

get_group(object, ...)

## S4 method for signature 'MultiAssayExperiment'
get_group(object)

get_metacell(object, ...)

## S4 method for signature 'SummarizedExperiment'
get_metacell(object, slot.name = c("metacell", "qMetacell"))

get_cc(object, ...)

## S4 method for signature 'SummarizedExperiment'
get_cc(object)

get_parentProtId(object, ...)
```

```
## S4 method for signature 'SummarizedExperiment'
get_parentProtId(object)

get_colID(object, ...)

## S4 method for signature 'SummarizedExperiment'
get_colID(object)

get_type(object, ...)

## S4 method for signature 'SummarizedExperiment'
get_type(object)

get_pkg_version(object, ...)

## S4 method for signature 'SummarizedExperiment'
get_pkg_version(object)
```

Arguments

<code>object</code>	An instance of class <code>SummarizedExperiment</code> .
<code>...</code>	Additional parameters
<code>slot.name</code>	The name of the slot dedicated to cell metadata to search. Default values are 'metacell' and 'qMetacell'

Value

See individual method description for the return value.

If exists, the slot value requested.

A `DataFrame` containing the adjacency matrix of the dataset

A `data.frame` containing the metadata of the dataset

A `data.frame` containing the metadata of the dataset

A `data.frame` containing the metadata of the dataset

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A `data.frame` containing the metadata of the dataset

A `data.frame` containing the metadata of the dataset

Examples

```
## -----
## Accessing slots from a MSnSet dataset
## -----
data(sub_R25)
```

```

se1 <- sub_R25[[1]]
parentProtId <- get_parentProtId(se1)
colID <- get_colID(se1)
type <- get_type(se1)
metacell <- get_metacell(se1)
conds <- get_group(sub_R25)

```

BuildColorStyles	<i>Build color style for DT tables</i>
------------------	--

Description

This function builds a list which is used for styling DT tables with the function `DT::styleEqual()`

Usage

```
BuildColorStyles(type)
```

Arguments

type	The type of dataset. Available values are protein and peptide
------	---

Value

A list

Examples

```
NULL
```

Build_enriched_qdata	<i>Builds enriched assay with cell metadata info</i>
----------------------	--

Description

If the cell metadata exists in the object of class `SummarizedExperiment`, then these information are added to the quantitative data so as to use styles with the functions of the package DT.

Usage

```
Build_enriched_qdata(obj)
```

Arguments

obj	An instance of the class <code>SummarizedExperiment</code>
-----	--

Value

A data.frame with new colums corresponding to the cell metadata (if exists)

Examples

NULL

color-legend	<i>Color legend for DaparToolshed</i>
--------------	---------------------------------------

Description

Shows a legend based on the tags in the package 'DaparToolshed'

Usage

```
custom_metacell_colors()

colorLegend_ui(id)

colorLegend_server(
  id,
  presentTags = reactive({
    NULL
  }),
  hide.white = TRUE
)

colorLegend(dataIn = SummarizedExperiment::SummarizedExperiment())
```

Arguments

- id A character(1) which is the id of the shiny module.
- presentTags A vector of character() which correspond to the tags.
- hide.white A boolean() to indicate whether the white cells must be hidden or not.
- dataIn An instance of the class SummarizedExperiment.

Value

- A vector
- NA
- NA
- A shiny app

Examples

```
if (interactive()) {  
  data(vdata)  
  shiny::runApp(colorLegend(vdata[[1]]))  
}
```

converters

Convert to enriched MultiAssayExperiment

Description

The resulting object is an instance of the MultiAssayExperiment class.

Usage

```
convert_to_mae(obj)  
  
MSnSet_to_mae(obj)  
  
matrix_to_mae(obj)  
  
df_to_mae(obj)  
  
Compute_CC(obj)  
  
QFeatures_to_mae(obj)  
  
SE_to_mae(obj)  
  
MAE_to_mae(obj)  
  
Check_se_Consistency(obj)  
  
list_to_se(ll)  
  
Check_List_consistency(ll)  
  
listOfLists_to_mae(obj, colData = NULL)  
  
listOfSE_to_mae(obj)  
  
Check_MSnSet_Consistency(obj)  
  
matrix_to_se(obj)  
  
df_to_se(obj)
```

MSnSet_to_se(obj)

Build_X_CC(se)

listOfMSnSet_to_mae(obj)

listOfmatrix_to_mae(obj)

listOfdf_to_mae(obj)

Arguments

obj	An object compliant with the formats accepted by omXplore
ll	A list
colData	A data.frame()
se	AN instance of the class SummarizedExperiment

Value

An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 An instance of SimpleList
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 A boolean(1)
 An enriched instance of the class SummarizedExperiment
 A boolean(1)
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 A boolean(1)
 An enriched instance of the class SummarizedExperiment
 An enriched instance of the class SummarizedExperiment
 An enriched instance of the class SummarizedExperiment
 An enriched instance of the class SummarizedExperiment
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment
 An enriched instance of the class MultiAssayExperiment

Examples

```
#-----
# Conversion of a MultiAssayExperiment instance
#-----
data(miniACC, package = "MultiAssayExperiment")
convert_to_mae(miniACC)
```

corrmatrix	<i>Displays a correlation matrix of the quantitative data of a numeric matrix.</i>
------------	--

Description

Displays a correlation matrix of the quantitative data of a numeric matrix.

Usage

```
omXplore_corrmatrix_ui(id)

omXplore_corrmatrix_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    1
  })
)

corrMatrix(data, rate = 0.5, showValues = FALSE)

omXplore_corrmatrix(dataIn, i)
```

Arguments

id	A character(1) which is the id of the shiny module.
dataIn	An instance of the class SummarizedExperiment
i	An integer which is the index of the assay in the param dataIn
data	An object of class 'matrix'
rate	The rate parameter to control the exponential law for the gradient of colors
showValues	A boolean which indicates whether to show values in the correlation plot.

Value

- NA
- NA
- A plot
- A shiny app

Examples

```
if (interactive()) {
  data(vdata)
  omXplore_corrmatrix(vdata, 1)
}
```

customChart	<i>Customised resetZoom Button of highcharts plots</i>
-------------	--

Description

Customised resetZoom Button of highcharts plots

Usage

```
customChart(
  hc,
  chartType = "scatter",
  zoomType = "None",
  width = 0,
  height = 0
)
```

Arguments

- | | |
|-----------|--|
| hc | A highcharter object |
| chartType | The type of the plot |
| zoomType | The type of the zoom (one of "x", "y", "xy", "None") |
| width | The width of the plot |
| height | The height of the plot |

Value

A highchart plot

Author(s)

Samuel Wieczorek

Examples

```
if (interactive()) {  
  library(highcharter)  
  hc <- highchart()  
  hc_chart(hc, type = "line")  
  hc_add_series(hc, data = c(29, 71, 40))  
  customChart(hc)  
}  
  
NULL
```

customExportMenu	<i>#' @title Customised contextual menu of highcharts plots</i>
------------------	---

Description

#' @title Customised contextual menu of highcharts plots

Usage

```
customExportMenu(hc, fname)
```

Arguments

hc	A highcharter object
fname	The filename under which the plot has to be saved

Value

A contextual menu for highcharts plots

Author(s)

Samuel Wiczorek

Examples

```
NULL
```

density-plot	<i>Displays a correlation matrix of the quantitative data of a numeric matrix.</i>
--------------	--

Description

Displays a correlation matrix of the quantitative data of a numeric matrix.

Usage

```
omXplore_density_ui(id)

omXplore_density_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    1
  }),
  pal.name = reactive({
    NULL
  })
)

densityPlot(data, conds = NULL, pal.name = NULL)

omXplore_density(dataIn, i)
```

Arguments

id	A character(1) which is the id of the shiny module.
dataIn	An instance of the class SummarizedExperiment
i	An integer which is the index of the assay in the param obj
pal.name	A character(1) which is the name of the palette from the package RColorBrewer::RColorBrewer from which the colors are taken. Default value is 'Set1'.
data	A data.frame() of quantitative data
conds	A vector indicating the name of each sample.

Value

NA
 NA
 A plot
 A shiny app

Examples

```

if (interactive()) {
  data(vdata)
  shiny::runApp(omXplore_density(vdata, 1))
}

if (interactive()) {
  data(vdata)
  qdata <- SummarizedExperiment::assay(vdata[[1]])
  conds <- get_group(vdata)
  densityPlot(qdata, conds)
}

```

ds-cc

*plots_cc_ui and plots_cc_server***Description**

A shiny Module.

Usage

```

omXplore_cc_ui(id)

omXplore_cc_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    NULL
  })
)

omXplore_cc(dataIn, i)

```

Arguments

<code>id</code>	A character(1) which is the id of the shiny module.
<code>dataIn</code>	An instance of SummarizedExperiment class
<code>i</code>	An integer which is the index of the assay in the param obj

Value

A shiny module

A shiny plot

A shiny module

A shiny app

A shiny app

Examples

```
if (interactive()) {
  data(vdata)
  shiny::runApp(omXplore_cc(vdata, 1))
}
```

ds-pca

my_PCA

Description

Process a PCA, using nipals or FactoMineR, on a quantitative dataset.

This method plots a bar plot which represents the distribution of the number of missing values (NA) per lines (ie proteins).

- wrapper_pca()
- plotPCA_Eigen_hc(): plots the eigen values of PCA with the highcharts library
- plotPCA_Eigen(): plots the eigen values of PCA
- plotPCA_Var()
- plotPCA_Ind()

Usage

```
my_PCA(
  X,
  scale.unit = TRUE,
  ncp = min(12, nrow(X) - 1, ncol(X)),
  ind.sup = NULL,
  quanti.sup = NULL,
  quali.sup = NULL,
  row.w = NULL,
  col.w = NULL,
  graph = FALSE,
  axes = c(1, 2),
  approach = "FM",
```

```

    gramschmidt = TRUE
  )

  omXplore_pca_ui(id)

  omXplore_pca_server(id, dataIn, i)

  omXplore_pca(dataIn, i)

  wrapper_pca(
    qdata,
    group,
    var.scaling = TRUE,
    ncp = NULL,
    approach = "FM",
    gramschmidt = TRUE
  )

  plotPCA_Eigen(res.pca)

  plotPCA_Var(res.pca, chosen.axes = c(1, 2))

  plotPCA_Ind(res.pca, chosen.axes = c(1, 2))

  plotPCA_Eigen_hc(res.pca)

```

Arguments

<code>X</code>	a <code>data.frame()</code> of quantitative data
<code>scale.unit</code>	See <code>FactoMineR::PCA()</code>
<code>ncp</code>	See <code>FactoMineR::PCA()</code>
<code>ind.sup</code>	See <code>FactoMineR::PCA()</code>
<code>quanti.sup</code>	See <code>FactoMineR::PCA()</code>
<code>quali.sup</code>	See <code>FactoMineR::PCA()</code>
<code>row.w</code>	See <code>FactoMineR::PCA()</code>
<code>col.w</code>	See <code>FactoMineR::PCA()</code>
<code>graph</code>	See <code>FactoMineR::PCA()</code>
<code>axes</code>	See <code>FactoMineR::PCA()</code>
<code>approach</code>	a string corresponding to the package to use for PCA (if no NA, default is "FM" for <code>FactoMineR</code>)
<code>gramschmidt</code>	A boolean indicating whether to use Gram-Schmidt orthogonalization or not.
<code>id</code>	A <code>character(1)</code> which is the id of the shiny module.
<code>dataIn</code>	An instance of the class <code>MultiAssayExperiment</code> .
<code>i</code>	An integer which is the index of the assay in the param obj

<code>qdata</code>	A <code>data.frame()</code> of quantitative data
<code>group</code>	A vector with the name of samples
<code>var.scaling</code>	A boolean indicating whether to scale the data or not
<code>res.pca</code>	The result of the function <code>FactoMineR::PCA()</code>
<code>chosen.axes</code>	See the parameter 'axes' of the function <code>factoextra::fviz_pca_var()</code>

Value

`res.pca` a "PCA" "list" object
`NA`
`NA`
 A shiny app
 The result of the function `FactoMineR::PCA()`
 A plot
 A plot
 A plot
 A plot

Author(s)

Samuel Wiczorek, Enora Fremy

Examples

```

if (interactive()) {
  data(vdata)
  obj <- vdata[[1]]
  res.pca <- my_PCA(SummarizedExperiment::assay(obj), approach = "FM")
  plotPCA_Eigen(res.pca)
  plotPCA_Var(res.pca)
  plotPCA_Eigen_hc(res.pca)
  plotPCA_Ind(res.pca)
}

if (interactive()) {
  data(vdata)
  library(shiny)
  library(dplyr)
  library(highcharter)
  # Replace missing values for the example
  sel <- is.na(SummarizedExperiment::assay(vdata, 1))
  SummarizedExperiment::assay(vdata[[1]])[sel] <- 0
  SummarizedExperiment::assay(vdata[[1]])[1, 1] <- NA
  omXplore_pca(vdata, 1)
}

if (interactive()) {

```

```

    data(vdata)
    obj <- vdata[[1]]
    res.pca <- wrapper_pca(qdata = SummarizedExperiment::assay(obj), group = get_group(obj))
    plotPCA_Eigen(res.pca)
    plotPCA_Var(res.pca)
    plotPCA_Eigen_hc(res.pca)
    plotPCA_Ind(res.pca)
  }

```

ds-view

*Bar plot of missing values per lines using highcharter.***Description**

This method plots a bar plot which represents the distribution of the number of missing values (NA) per lines (i.e. proteins).

Usage

```

view_dataset_ui(id)

view_dataset_server(
  id,
  dataIn = reactive({
    NULL
  }),
  addons = list(),
  verbose = FALSE
)

view_dataset(dataIn = NULL, addons = NULL)

```

Arguments

id	A character(1) for the 'id' of the shiny module. It must be the same as for the '*_ui' function.
dataIn	An instance of the class MultiAssayExperiment.
addons	A list to configure the other shiny apps to integrate. Each item correspond to one package: - the name of the slot is the name of the package - the content of the slot is a vector composed of the generic name of the shiny app. Each of the apps listed here must be an exported app of the package. For example, given the value addons = list(testPkg = c('foo', 'foo2')). That means that the package called "testPkg" must provide the four functions: foo1_ui(), foo1_server() and foo2_ui(), foo2_server()
verbose	A boolean for verbose mode. Default is FALSE.

Details

- distribution of the missing values per line,
- a bar plot which represents the distribution of the number of missing values (NA) per lines (i.e. proteins) and per conditions,
- Histogram of missing values.
- Variance : Builds a densityplot of the CV of entities in numeric matrix. The CV is calculated for each condition present in the dataset (see the slot 'Condition' in the colData() DataFrame)
- Heatmap:

The function `heatmapD()`

The function `[]` is inspired from the function 'heatmap.2' that displays a numeric matrix. For more information, please refer to the help of the heatmap.2 function.

Value

NA

NA

NA

A shiny application which wraps the functions `view_dataset_ui()` and the `view_dataset_server()`

Missing values

#' - distribution of the missing values per line,

- a bar plot which represents the distribution of the number of missing values (NA) per lines (ie proteins) and per conditions,
- Histogram of missing values.

Author(s)

Samuel Wieczorek, Enora Fremy

Examples

```
if (interactive()) {
  library(shiny)
  library(omXplore)
  data(vdata)
  addons <- list(omXplore = c("extFoo1", "extFoo2"))
  runApp(omXplore::view_dataset(vdata, addons))

  omXplore::view_dataset(vdata)
}

if (interactive()) {
  data(vdata)
  view_dataset(vdata)
```

```
}
```

```
external_app
```

```
External module example
```

Description

Example for an external shiny module, well structured to be run within a workflow for MagellanNTK

Usage

```
extFoo1_ui(id)

extFoo1_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    NULL
  })
)

extFoo1(dataIn, i)

extFoo2_ui(id)

extFoo2_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    NULL
  })
)

extFoo2(dataIn, i)
```

Arguments

id	A character(1) which is the id of the shiny module.
dataIn	An object of instance MultiAssayExperiment
i	An integer which is the index of the assay in the param obj

Value

NA
 NA
 NA
 A shiny app
 NA
 NA
 A shiny app

Examples

```
if (interactive()) {
  data(vdata)
  app1 <- extFoo1(vdata, 1)
  app2 <- extFoo2(vdata, 1)
  shiny::runApp(app1)
  shiny::runApp(app2)
}
```

FormatDataForDT

Constructs a dataset suitable to use with the module format_DT.

Description

This function builds the skeleton of a dataset which can be used by the module formatDT. It creates additional columns to be used to style the table. to colors cells.

Usage

```
FormatDataForDT(se, digits = 2)
```

Arguments

se	An instance of the class SummarizedExperiment
digits	An 'integer(1)' to specify the number of digits to display in the tables for numerical values. Default is 2.

Value

A data.frame

format_DT	<i>formatDT_ui and formatDT_server</i>
-----------	--

Description

A shiny Module.

See DT package homepage for more details about styling tables. If no style is precised, this module show the raw data. If any style is given, then the dataset must be well configured (I.e. it must contain the correct columns)

Usage

```
formatDT_ui(id)

formatDT_server(
  id,
  data = reactive({
    NULL
  }),
  data_nostyle = reactive({
    NULL
  }),
  withDLBtns = FALSE,
  showRownames = FALSE,
  dt_style = reactive({
    NULL
  }),
  filename = "Prostar_export",
  selection = "single"
)

formatDT(data)
```

Arguments

id	shiny id
data	A data.frame
data_nostyle	A data.frame() to be bind to the main data with no custom style
withDLBtns	A boolean to indicate whether to display download buttons or not.
showRownames	A boolean to indicate whether to show rownames.
dt_style	A list composed of: • data : a data.frame • colors : a named vector
filename	A character(1) which is the default filename for download.
selection	A character(1) which indicates the type of selection. Default is 'single'.

Value

NA

NA

NA

NA

Examples

```
if (interactive()) {  
  data(vdata)  
  formatDT(vdata)  
}
```

GetPkgVersion*Package version*

Description

Gets the version number of a package

Usage

```
GetPkgVersion(pkg)
```

Arguments

pkg The name of the package

Value

A character(1) with the name of the package and its version number.

Examples

```
GetPkgVersion("omXplore")
```

globals	<i>Global variables</i>
---------	-------------------------

Description

Defines the global variables for the package omXplore

Usage

```
globals()
```

Value

A list

Examples

```
globals()
```

intensity-plots	<i>Displays different intensity plots.</i>
-----------------	--

Description

Displays different intensity plots.

Usage

```
omXplore_intensity_ui(id)

omXplore_intensity_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    1
  }),
  track.indices = reactive({
    NULL
  }),
  remoteReset = reactive({
    NULL
  }),
  is.enabled = reactive({
```

```

      TRUE
    })
  )

omXplore_intensity(dataIn, i = NULL, withTracking = FALSE)

boxPlot(dataIn, conds, legend = NULL, pal = NULL, subset = NULL)

violinPlot(data, conds, subset = NULL, pal.name = "Set1")

```

Arguments

id	A character(1) which is the id of the shiny module.
dataIn	xxxx
i	An integer which is the index of the assay in the param obj
track.indices	A vector of integers which are the indices of lines to track.
remoteReset	An integer to activate the reset functions
is.enabled	A boolean that indicates whether the widgets should be enabled or disabled. Default is TRUE
withTracking	A boolean(1) indicating whether the tracking option is activated or not.
conds	A vector indicating the name of each sample.
legend	A vector of the conditions (one condition per sample).
pal	A basis palette for the boxes which length must be equal to the number of unique conditions in the dataset.
subset	A integer() vector of index indicating the indices of rows in the dataset to highlight
data	xxxx
pal.name	A character(1) which is the name of the palette from the package RColorBrewer::RColorBrewer from which the colors are taken. Default value is 'Set1'.

Value

NA
 NA
 A shiny app
 A boxplot
 A violin plot

Author(s)

Samuel Wieczorek, Anais Courtier, Enora Fremy

Examples

```
if (interactive()) {
  data(vdata)
  shiny::runApp(omXplore_intensity(vdata, 1))

  data(sub_R25)
  conds <- legend <- SummarizedExperiment::colData(sub_R25)$group
  pal <- ExtendPalette(length(unique(conds)))
  boxPlot(sub_R25[[1]], conds, legend, pal, seq_len(10))

  shiny::runApp(omXplore_intensity(sub_R25, 1, withTracking = TRUE))
}
```

`is.listOf`*Checks the class of a list's slots*

Description

Checks if all slots of the given list are of the same class.

Usage

```
is.listOf(object, obj.class = NULL)
```

Arguments

<code>object</code>	A list
<code>obj.class</code>	The name of the class to search in items of the list.

Value

A character(1) with the name of the package or NULL

Examples

```
ll <- as.list(LETTERS[1:3])
is.listOf(ll, "data.frame")
is.listOf(ll, "character")
```

omXplore-modules	<i>Shiny modules used by omXplore</i>
------------------	---------------------------------------

Description

These functions are relative to external modules that can be added into omXplore UI:

- `listShinyApps()`: Show the shiny modules recognized by omXplore and ready to be integrated in the UI of the function `view_dataset()`
- `listPlotModules()`: Show the shiny modules function names (only prefixes) recognized by omXplore and ready to use in the UI.
- `addModules()`: Add external shiny module(s) to the R global environment in such a way (specific prefix renaming of the functions) that it can be discovered by the function `view_dataset()` of the package omXplore during its launch.

Usage

```
addModules(addons = list())
```

```
listShinyApps(location = "both")
```

```
listPlotModules(location = "both")
```

Arguments

<code>addons</code>	A list in which each item: • is named by the name of a package containing the modules to add, • contains the name of the shiny modules to integrate (without <code>'_ui'</code> nor <code>'_server'</code> suffixes)
<code>location</code>	A character(<code>0</code>) to indicate which modules to list. Available values are: <code>'builtin'</code> , <code>'external'</code> and <code>'both'</code> (default).

Value

NA

A vector

A vector

Examples

```
listShinyApps()
listPlotModules()
```

```
#####
# Integration of a module in the package 'mypackage'
#####
```

```
addons <- list(omXplore = c("extFoo1", "extFoo2"))
addModules(addons)
```

omXplore_heatmap	<i>Displays a correlation matrix of the quantitative data of a numeric matrix.</i>
------------------	--

Description

This function is a wrapper to `heatmap.2()` that displays assay data in an instance of `SummarizedExperiment`. For more details, see `heatmap.2()`.

Usage

```
omXplore_heatmap_ui(id)

omXplore_heatmap_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    NULL
  })
)

omXplore_heatmap(dataIn, i)

heatmapD(
  qdata,
  conds,
  distance = "euclidean",
  cluster = "complete",
  dendro = FALSE
)

mv.heatmap(
  x,
  col = grDevices::heat.colors(100),
  srtCol = NULL,
  labCol = NULL,
  labRow = NULL,
  key = TRUE,
  key.title = NULL,
  main = NULL,
  ylab = NULL
```

```

)

heatmapForMissingValues(
  x,
  col = NULL,
  srtCol = NULL,
  labCol = NULL,
  labRow = NULL,
  key = TRUE,
  key.title = NULL,
  main = NULL,
  ylab = NULL
)

```

Arguments

id	A character(1) which is the id of the shiny module.
dataIn	An instance of a class MultiAssayExperiment.
i	An integer which is the index of the assay in the param obj
qdata	A data.frame() of quantitative data.
conds	A vector indicating the name of each sample.
distance	The distance used by the clustering algorithm to compute the dendrogram.
cluster	the clustering algorithm used to build the dendrogram.
dendro	A boolean to indicate fi the dendrogram has to be displayed
x	A matrix or array containing the quantitative data.
col	Colors used for the image. Defaults to heat colors (heat.colors).
srtCol	Angle of column conds, in degrees from horizontal
labCol	Character vectors with column conds to use.
labRow	Character vectors with row conds to use.
key	Logical indicating whether a color-key should be shown.
key.title	Main title of the color key. If set to NA no title will be plotted.
main	Main title; default to none.
ylab	y-axis title; default to none.

Value

```

NA
NA
A shiny app
A heatmap
A heatmap
A heatmap

```

Author(s)

Florence Combes, Samuel Wiczorek, Enora Fremy

Examples

```
if (interactive()) {
  data(vdata)
  omXplore_heatmap(vdata, 1)
}
```

omXplore_tabExplorer *Explore MultiAssayExperiment objects.*

Description

Explore MultiAssayExperiment objects.

Usage

```
omXplore_tabExplorer_ui(id)

omXplore_tabExplorer_server(
  id,
  dataIn = reactive({
    NULL
  }),
  i = reactive({
    NULL
  }),
  digits = reactive({
    3
  })
)

omXplore_tabExplorer(dataIn, i)
```

Arguments

id	A character(1) which is the id of the shiny module.
dataIn	An instance of the class MultiAssayExperiment
i	An integer which is the index of the assay in the param obj
digits	An integer for the number of digits shown in the table

Value

NA
 NA
 NA
 A shiny app

Examples

```
if (interactive()) {
  data(vdata)
  shiny::runApp(omXplore_tabExplorer(vdata, 1))
}

NULL
```

 palette

Palette for samples.

Description

Builds a vector of #conditions colors for a set of samples. One color is given for a given condition. This function extends a base palette from the package [RColorBrewer::RColorBrewer](#) to 'n' colors. The colors in the returned palette are always in the same order

Usage

```
SampleColors(conds, pal.name = "Set1")

ExtendPalette(n, pal.name = "Set1")

GetColorsForConditions(conds, pal = NULL)
```

Arguments

conds	A <code>character()</code> of conditions. The length of the vector is the number of samples in the dataset.
pal.name	A <code>character(1)</code> which is the name of the palette from the package RColorBrewer::RColorBrewer from which the colors are taken. Default value is 'Set1'.
n	The number of desired colors in the palette
pal	A vector of HEX color code that form the basis palette from which to build the complete color vector for the conditions.

Value

A vector

A vector

A vector

Examples

```
if (interactive()) {
  #-----
  # Builds a palette for a dataset with 3 conditions
  # of 3 samples each.
  #-----

  conds <- c(rep("A", 3), rep("B", 3), rep("C", 3))
  SampleColors(conds)
  SampleColors(conds, "Dark2")

  #-----
  # Extend the default palette to 12 colors
  #-----

  ExtendPalette(12)

  data(vdata)
  conds <- get_group(vdata)
  GetColorsForConditions(conds, ExtendPalette(2))
}
```

pep_prot_CC

Display a CC

Description

Display a CC

Connected Components infos

Usage

buildGraph(cc = NULL, meta = NULL)

display.CC.visNet(g = NULL, layout = "layout_with_fr")

plotCCJitter(df, clickFunction = NULL)

GetCCInfos(cc)

Arguments

<code>cc</code>	A list of connected component
<code>meta</code>	A <code>data.frame()</code>
<code>g</code>	An instance of a graph
<code>layout</code>	A <code>character(1)</code> which is the layout used in <code>visNetwork</code> . Default value is <code>'layout_with_fr'</code>
<code>df</code>	A <code>data.frame()</code>
<code>clickFunction</code>	A JS function to determine the behaviour of a click

Value

A list

A plot

A plot

A list of three items:

- `One_One`: the number of cc composed of one protein and one peptide
- `One_Multi`: the number of cc composed of one protein and several peptides
- `Multi_Multi`: the number of cc composed of several proteins and several (shared) peptides.

Author(s)

Thomas Burger, Samuel Wiczorek

Examples

```
if (interactive()) {
  data(sub_R25)
  se <- sub_R25[[1]]
  g <- buildGraph(get_cc(se)[[1]])
  display.CC.visNet(g)
}

if (interactive()) {
  data(sub_R25)
  GetCCInfos(get_cc(sub_R25[[1]]))
}
```

pkgs.require2	<i>Loads packages</i>
---------------	-----------------------

Description

Checks if a package is available to load it

Usage

```
pkgs.require2(ll.deps)
```

Arguments

ll.deps A character() vector which contains packages names

Value

NA

Author(s)

Samuel Wieczorek

Examples

```
pkgs.require2("omXplore")
```

plot-variance	<i>Variance plot</i>
---------------	----------------------

Description

A shiny module which plots the variance of samples

Usage

```
omXplore_variance_ui(id)
```

```
omXplore_variance_server(id, dataIn, i, pal.name = NULL)
```

```
CVDist(dataIn, conds, pal.name = NULL)
```

```
omXplore_variance(dataIn, i)
```

Arguments

id	A character(1) which is the id of the shiny module.
dataIn	An matrix
i	An integer which is the index of the assay in the param obj
pal.name	A character(1) which is the name of the palette from the package RColorBrewer::RColorBrewer from which the colors are taken. Default value is 'Set1'.
conds	A vector indicating the name of each sample.

Value

NA
 NA
 A plot
 A shiny app

Examples

```
if (interactive()) {
  data(vdata)
  shiny::runApp(omXplore_variance(vdata, 1))
}
```

plots_tracking *plots_tracking_ui and plots_tracking_server*

Description

This shiny module provides a tool to select

Usage

```
plots_tracking_ui(id)

plots_tracking_server(
  id,
  dataIn = reactive({
    NULL
  }),
  remoteReset = reactive({
    NULL
  }),
  is.enabled = reactive({
    TRUE
  })
)
```

```
)
plots_tracking(obj)
```

Arguments

id	shiny id
remoteReset	A boolean(1) which indicates whether to show the 'Reset' button or not.
is.enabled	xxx
obj	An instance of the class MultiAssayExperiment

Value

NA

A list (same structure as the parameter params)

A shiny app

Examples

```
if (interactive()) {
  data(vdata)
  shiny::runApp(plots_tracking(vdata[[1]]))
}

NULL
```

Prostar-1x-compatible *Convert datasets exported by the package Prostar*

Description

Convert datasets exported by the package Prostar

Usage

```
SE_Compatibility_with_Prostar_1x(obj, se)

MAE_Compatibility_with_Prostar_1x(obj, mae)
```

Arguments

obj	An instance of the class MSnSet
se	An instance of the class SummarizedExperiment
mae	An instance of the class MultiAssayExperiment

Value

An enriched instance of the class SummarizedExperiment
An enriched instance of the class MultiAssayExperiment

Examples

```
data(sub_R25)
```

q_metadata	<i>Quantitative metadata vocabulary for entities</i>
------------	--

Description

This function gives the vocabulary used for the quantitative metadata of each entity in each condition.

Usage

```
metacell.def(level)

Parent(level, node = NULL)

Children(level, parent = NULL)

GetMetacellTags(metacells = NULL, level = NULL, onlyPresent = FALSE)
```

Arguments

level	A string corresponding to the type of object
node	The name of the node for which one wants its parent
parent	The name of the parent node
metacells	A data.frame() representing the cell metadata
onlyPresent	A boolean(1)

Value

A data.frame containing the different tags and corresponding colors for the level given in parameter
A list
A vector
A vector
A vector

Glossary

Peptide-level vocabulary

└ 'Any' |||└ 1.0 'Quantified' ||||└ 1.1 "Quant. by direct id" (color 4, white) ||||└ 1.2 "Quant. by recovery" (color 3, lightgrey) |||└ 2.0 "Missing" (no color) ||||└ 2.1 "Missing POV" (color 1) ||||└ 2.2 'Missing MEC' (color 2) |||└ 3.0 'Imputed' ||||└ 3.1 'Imputed POV' (color 1) |||└ 3.2 'Imputed MEC' (color 2)

Protein-level vocabulary: └ 'Any' |||└ 1.0 'Quantified' ||||└ 1.1 "Quant. by direct id" (color 4, white) ||||└ 1.2 "Quant. by recovery" (color 3, lightgrey) |||└ 2.0 "Missing" ||||└ 2.1 "Missing POV" (color 1) ||||└ 2.2 'Missing MEC' (color 2) |||└ 3.0 'Imputed' ||||└ 3.1 'Imputed POV' (color 1) ||||└ 3.2 'Imputed MEC' (color 2) |||└ 4.0 'Combined tags' (color 3bis, lightgrey)

Conversion to the glossary

A generic conversion

Conversion for Proline datasets

Conversion from Maxquant datasets

Author(s)

Thomas Burger, Samuel Wieczorek

Samuel Wieczorek

Examples

```
if (interactive()) {
  metacell.def("protein")
  metacell.def("peptide")
}

Parent("protein", "Missing")
Parent("protein", "Missing POV")
Parent("protein", c("Missing POV", "Missing MEC"))
Parent("protein", c("Missing", "Missing POV", "Missing MEC"))

Children("protein", "Missing")
Children("protein", "Missing POV")
Children("protein", c("Missing POV", "Missing MEC"))
Children("protein", c("Missing", "Missing POV", "Missing MEC"))
data(vdata)
metacells <- get_metacell(vdata[[1]])
level <- get_type(vdata[[1]])
GetMetacellTags(metacells, level)
```

sub_R25	<i>Feature example data</i>
---------	-----------------------------

Description

sub_R25 is a protein subset of the dataset 'Exp1_R25_pept' in the package DAPARdata.

Format

An instance of the class MultiAssayExperiment

Value

An enriched instance of the class MultiAssayExperiment

Source

sub_R25 was built from the source code available in `inst/scripts/build_datasets.R`

The DAPARdata package: <https://github.com/edyp-lab/DAPARdata>

vdata	<i>Feature example data</i>
-------	-----------------------------

Description

vdata is a small object for testing and demonstration.

Format

An instance of the class MultiAssayExperiment

Value

An enriched instance of the class MultiAssayExperiment

Source

vdata was built from the source code available in `inst/scripts/build_datasets.R`

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