Package 'notameViz'

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Type Package

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Description Provides visualization functionality for untargeted LC-MS metabolomics research. Includes quality control visualizations, feature-wise visualizations and results visualizations.

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Contents

`manhattan_plot` *Manhattan plot*

Description

Draws a (directed) Manhattan plot of p-values and versus e.g. retention time or mass-to-charge ratio. If effect size and direction is supplied, the - log10(p-value) on the y-axis will be multiplied by the direction (sign) of the effect, so part of the points will "drop" from the p = 1 (-log10(p) = 0) line. This results in a so-called directed Manhattan plot.

Usage

```
manhattan_plot(
  object,
  x,
  p,
  effect = NULL,
  p_fdr = NULL,
  color = NULL,
  p_breaks = c(0.05, 0.01, 0.001, 1e-04),
  fdr_limit = 0.05,
  x_lim = NULL,
  y_lim = NULL,
  color_scale = getOption("notame.color_scale_con"),
  title = "Manhattan plot",
  subtitle = NULL,
  ...
)
```

Arguments

`object`	a `SummarizedExperiment` object or a data frame like object. Feature data is used.
`x, p`	the column names of x-axis and p-values
`effect`	column name of effect size (should have negative and positive values).
`p_fdr`	column name of FDR corrected p-values, used to draw a line showing the fdr-corrected significance level
`color`	column name used to color the plots
`p_breaks`	a numerical vector of the p_values to show on the y-axis
`fdr_limit`	the significance level used in the experiment
`x_lim, y_lim`	numerical vectors of length 2 for manually setting the axis limits
`color_scale`	the color scale as returned by a ggplot function
`title, subtitle`	the title and subtitle of the plot
`...`	parameters passed to `geom_point`, such as shape and alpha values. New aesthetics can also be passed using `mapping = aes(...)`.

Value

A ggplot object.

Examples

```
data(toy_notame_set, package = "notame")
# naturally, this looks messy as there are not enough p-values
lm_results <- notameStats::perform_lm(notame::drop_qcs(toy_notame_set),
  formula_char = "Feature ~ Group")
lm_data <- dplyr::left_join(as.data.frame(rowData(toy_notame_set)),
  lm_results)
# Traditional Manhattan plot from data frame
manhattan_plot(lm_data,
  x = "Average_Mz",
  p = "GroupB.p.value", p_fdr = "GroupB.p.value_FDR",
  fdr_limit = 0.1
)
# Directed Manhattan plot from SummarizedExperiment
with_results <- notame::join_rowData(toy_notame_set, lm_results)
manhattan_plot(with_results,
  x = "Average_Mz", effect = "GroupB.estimate",
  p = "GroupB.p.value", p_fdr = "GroupB.p.value_FDR",
  fdr_limit = 0.1
)
```

---

mz_rt_plot *Plot m/z vs retention time plot (cloud plot)*

Description

Plots a scatter plot of results of statistical tests, where each point represents a feature. The plot has retention time on x-axis, m/z on y-axis and the size of the points is scaled based on p-value

Usage

```
mz_rt_plot(
  object,
  p_col = NULL,
  p_limit = NULL,
  mz_col = NULL,
  rt_col = NULL,
  color = NULL,
  title = "m/z vs retention time",
  subtitle = NULL,
  color_scale = getOption("notame.color_scale_con"),
  all_features = FALSE,
  ...
)
```

Arguments

object	a SummarizedExperiment object or a data frame. Feature data is used. If x is a data frame, it is used as is.
p_col	the column name containing p-values. This is used to scale the size of the points.
p_limit	numeric, limits plotted features by p-values. If NULL, plots all features.

mz_col, rt_col	the column names for m/z and retention time. If NULL, automatic detection is attempted.
color	the column name used to color the points
title	The plot title
subtitle	The plot subtitle
color_scale	color scale as returned by a ggplot function. Defaults to current continuous color scale.
all_features	logical, should all features be retained? Should be used only if x is a SummarizedExperiment object.
...	parameters passed to geom_point, such as shape and alpha values. New aesthetics can also be passed using mapping = aes(...).

Value

A ggplot object.

Examples

```
data(toy_notame_set, package = "notame")
# Compute results from a linear model
lm_results <- notameStats::perform_lm(toy_notame_set,
  formula_char = "Feature ~ Group")
with_results <- notame::join_rowData(toy_notame_set, lm_results)

# Plot from the SummarizedExperiment object
# automatically facet by analytical mode in variable Split
mz_rt_plot(with_results, p_col = "GroupB.p.value", color = "GroupB.estimate")

# Plot the results from the results dataframe
lm_data <- dplyr::left_join(as.data.frame(rowData(toy_notame_set)),
                            lm_results)
mz_rt_plot(lm_data, p_col = "GroupB.p.value", color = "GroupB.estimate")
```

---

plot_dendrogram *Sample dendrogram*

Description

Draws a dendrogram of a hierarchical clustering applied to the samples of an experiment.

Usage

```
plot_dendrogram(
  object,
  all_features = FALSE,
  color,
  dist_method = "euclidean",
  clust_method = "ward.D2",
  center = TRUE,
  scale = "uv",
```

```
  title = "Dendrogram of hierarchical clustering",
  subtitle = NULL,
  color_scale = getOption("notame.color_scale_dis"),
  assay.type = NULL
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
color	character, name of the column used for coloring the sample labels
dist_method	distance method used in clustering as in dist
clust_method	method used in clustering as in hclust
center	logical, should the data be centered?
scale	scaling used, as in prep. Default is "uv" for unit variance
title	The plot title
subtitle	The plot subtitle
color_scale	the color scale as returned by a ggplot function.
assay.type	character, assay to be used in case of multiple assays

Value

A ggplot object.

See Also

dist hclust

Examples

```
data(toy_notame_set, package = "notame")
plot_dendrogram(toy_notame_set, color = "Group")
```

---

plot_dist_density *Plot distance density*

Description

Plot density of distances between samples in QC samples and actual samples.

Usage

```
plot_dist_density(
  object,
  all_features = FALSE,
  dist_method = "euclidean",
  center = TRUE,
  scale = "uv",
  color_scale = getOption("notame.color_scale_dis"),
  fill_scale = getOption("notame.fill_scale_dis"),
  title = paste("Density plot of", dist_method, "distances between samples"),
  subtitle = NULL,
  assay.type = NULL
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
dist_method	method for calculating the distances, passed to dist
center	logical, should the data be centered?
scale	scaling used, as in prep Default is "uv" for unit variance
color_scale	a scale for the color of the edge of density curves, as returned by a ggplot function
fill_scale	a scale for the fill of the density curves, as returned by a ggplot function
title	the plot title
subtitle	the plot subtitle
assay.type	character, assay to be used in case of multiple assays

Value

A ggplot object.

See Also

dist

Examples

```
data(toy_notame_set, package = "notame")
plot_dist_density(toy_notame_set)
# Drift correction tightens QCs together
plot_dist_density(notame::correct_drift(toy_notame_set))
```

`plot_effect_heatmap` *Heatmap of effects between variables, such as correlations*

Description

Draws a heatmap of e.g. correlations between variables (see perform_correlation_tests). It is possible to draw only the lower triangular of the heatmap, order rows and columns with hierarchical clustering, and add circles for p-values.

Usage

```
plot_effect_heatmap(
  data,
  x,
  y,
  effect,
  p = NULL,
  p_limit = 0.1,
  point_size_range = c(1, 6),
  log2_effect = FALSE,
  discretize_effect = FALSE,
  breaks = 5,
  clustering = TRUE,
  dist_method = "euclidean",
  clust_method = "ward.D2",
  lower_tri = FALSE,
  reverse_y = TRUE,
  use_coord_fixed = TRUE,
  symmetric_aspect_ratio = TRUE,
  title = NULL,
  subtitle = NULL,
  fill_scale = NA
)
```

Arguments

`data`	a data frame with x and y variables and the effect
`x, y`	the column names of data with the x and y variables
`effect`	the column name of the effect, e.g. correlation
`p`	optional, the column name with p-values. If provided, points that scale by p-value are drawn on top of the heatmap tiles
`p_limit`	numeric, only p-values below the limit are plotted as points
`point_size_range`	a numeric vector of length 2. The upper and lower limits for the point sizes. This needs to be adjusted to make the point size look good when compared to the tiles
`log2_effect`	logical, whether the effect should be plotted on a logarithmic scale (in case of fold change etc.)

`discretize_effect`
: logical, whether the effect range should be divided into discrete levels instead of using a continuous scale. Can sometimes make patterns more visible, but the hard limits can blur the big picture as well.

`breaks`
: if `discretize_effect = TRUE`, either the number of breaks or the points where to cut for the levels, see `cut`

`clustering`
: logical, whether the order of rows and columns should be ordered by hierarchical clustering?

`dist_method`
: distance method used in clustering, see `dist`

`clust_method`
: clustering method used in clustering, see `hclust`

`lower_tri`
: logical, should only the lower triangular be plotted?

`reverse_y`
: logical, if `clustering = FALSE`, `lower_tri = FALSE`, should the order of the y-axis be reversed so that the diagonal is from top left to bottom right?

`use_coord_fixed`
: logical, should the heatmap tiles be squares? If yes, this uses `coord_fixed`

`symmetric_aspect_ratio`
: logical, should the plot panel be a square? If yes, uses ggplot2::theme(aspect.ratio = 1).

`title, subtitle`
: the title and subtitle of the plot

`fill_scale`
: fill scale for the heatmap as returned by a ggplot function. Set to NA to choose the appropriate scale based on the class of the effect variable.

Details

All missing effects between variables are replaced by 0 before clustering, since `hclust` can't deal with missing values.

Value

A ggplot object.

See Also

`cut` for discretizing the effect, `dist` for distance calculation for clustering, `hclust` for hierarchical clustering.

Examples

```
data(toy_notame_set, package = "notame")
# Compute correlations between variables
correlations <- notameStats::perform_correlation_tests(toy_notame_set,
  x = rownames(toy_notame_set),
  duplicates = TRUE
)

# Minimal example
plot_effect_heatmap(correlations,
x = "X", y = "Y", effect = "Correlation_coefficient")

# Lower triangular with discrete effect and p-value dots
plot_effect_heatmap(correlations,
  x = "X", y = "Y", effect = "Correlation_coefficient",
```

```
  p = "Correlation_P", point_size_range = c(2, 8),
  discretize_effect = TRUE, breaks = 7, lower_tri = TRUE
)
```

`plot_injection_lm` *Estimate the magnitude of drift*

Description

Plots histograms of p-values from linear regression model, where each feature is predicted by injection order alone. The expected uniform distribution is represented by a dashed red line.

Usage

```
plot_injection_lm(object, all_features = FALSE, assay.type = NULL)
```

Arguments

`object`	a `SummarizedExperiment` object
`all_features`	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
`assay.type`	character, assay to be used in case of multiple assays

Value

A ggplot object.

See Also

`plot_p_histogram`

Examples

```
data(toy_notame_set, package = "notame")
plot_injection_lm(toy_notame_set)
```

`plot_pca` *PCA scatter plot*

Description

Computes PCA using one of the methods provided in the Bioconductor package pcaMethods and plots the two first principal components.

Usage

```
plot_pca(
  object,
  pcs = c(1, 2),
  all_features = FALSE,
  center = TRUE,
  scale = "uv",
  color = NULL,
  shape = color,
  label = NULL,
  density = FALSE,
  title = "PCA",
  subtitle = NULL,
  color_scale = NA,
  shape_scale = getOption("notame.shape_scale"),
  fill_scale = getOption("notame.fill_scale_dis"),
  text_base_size = 14,
  point_size = 2,
  assay.type = NULL,
  ...
)
```

Arguments

object	a SummarizedExperiment object
pcs	numeric vector of length 2, the principal components to plot
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
center	logical, should the data be centered prior to PCA? (usually yes)
scale	scaling used, as in prep. Default is "uv" for unit variance
color	character, name of the column used for coloring the points. Set to NULL for black color.
shape	character, name of the column used for shape. Set to NULL for uniform round shapes.
label	character, name of the column used for point labels
density	logical, whether to include density plots to both axes. The density curves will be split and colored by the 'color' variable.
title, subtitle	the titles of the plot
color_scale	the color scale as returned by a ggplot function. Set to NA to choose the appropriate scale based on the class of the coloring variable.
shape_scale	the shape scale as returned by a ggplot function
fill_scale	the fill scale used for density curves. If a continuous variable is used as color, density curve will be colorless.
text_base_size	numeric, base size for text
point_size	numeric, size of the points
assay.type	character, assay to be used in case of multiple assays
...	additional arguments passed to pca

Value

A ggplot object. If `density` is `TRUE`, the plot will consist of multiple parts and is harder to modify.

See Also

`pca`

Examples

```
data(toy_notame_set, package = "notame")
plot_pca(toy_notame_set, color = "Injection_order", shape = "Group")
```

`plot_pca_arrows` *PCA plot with arrows*

Description

Plots changes in PCA space according to time. All the observations of a single subject are connected by an arrow ending at the last observation.

Usage

```
plot_pca_arrows(
  object,
  pcs = c(1, 2),
  all_features = FALSE,
  center = TRUE,
  scale = "uv",
  color,
  time,
  subject,
  alpha = 0.6,
  arrow_style = arrow(),
  title = "PCA changes",
  subtitle = NULL,
  color_scale = getOption("notame.color_scale_dis"),
  text_base_size = 14,
  line_width = 0.5,
  assay.type = NULL,
  ...
)
```

Arguments

`object`	a `SummarizedExperiment` object
`pcs`	numeric vector of length 2, the principal components to plot
`all_features`	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
`center`	logical, should the data be centered prior to PCA? (usually yes)

scale	scaling used, as in prep. Default is "uv" for unit variance
color	character, name of the column used for coloring the arrows
time	character, name of the column containing timepoints
subject	character, name of the column containing subject identifiers
alpha	numeric, value for the alpha parameter of the arrows (transparency)
arrow_style	a description of arrow heads, the size and angle can be modified, see ?arrow
title, subtitle	the titles of the plot
color_scale	the color scale as returned by a ggplot function
text_base_size	the base size of the text
line_width	the width of the arrows
assay.type	character, assay to be used in case of multiple assays
...	additional arguments passed to pca

Value

A ggplot object.

See Also

pca

Examples

```
data(toy_notame_set, package = "notame")
plot_pca_arrows(notame::drop_qcs(toy_notame_set), color = "Group",
  time = "Time", subject = "Subject_ID")
# If the sample size is large, plot groups separately
plot_pca_arrows(notame::drop_qcs(toy_notame_set), color = "Group",
                time = "Time", subject = "Subject_ID") +
  facet_wrap(~Group)
```

---

plot_pca_hexbin *PCA hexbin plot*

Description

Computes PCA using one of the methods provided in the Bioconductor package pcaMethods and plots the two first principal components as hexagonal bins, where the value of the coloring variable is summarised for each bin, by default as the mean of the values inside the bin.

Usage

```
plot_pca_hexbin(
  object,
  pcs = c(1, 2),
  all_features = FALSE,
  center = TRUE,
  scale = "uv",
  fill = "Injection_order",
  summary_fun = "mean",
  bins = 10,
  title = "PCA",
  subtitle = NULL,
  fill_scale = getOption("notame.fill_scale_con"),
  assay.type = NULL,
  ...
)
```

Arguments

object	a SummarizedExperiment object
pcs	numeric vector of length 2, the principal components to plot
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
center	logical, should the data be centered prior to PCA? (usually yes)
scale	scaling used, as in prep. Default is "uv" for unit variance
fill	character, name of the column used for coloring the hexagons
summary_fun	the function used to compute the value for each hexagon
bins	the number of bins in x and y axes
title, subtitle	the titles of the plot
fill_scale	the fill scale as returned by a ggplot function
assay.type	character, assay to be used in case of multiple assays
...	additional arguments passed to pca

Value

A ggplot object.

See Also

pca

Examples

```
data(toy_notame_set, package = "notame")
plot_pca_hexbin(toy_notame_set)
```

`plot_pca_loadings` *PCA loadings plot*

Description

Computes PCA using one of the methods provided in the Bioconductor package pcaMethods and plots the loadings of first principal components.

Usage

```
plot_pca_loadings(
  object,
  pcs = c(1, 2),
  all_features = FALSE,
  center = TRUE,
  scale = "uv",
  n_features = c(10, 10),
  title = "PCA loadings",
  subtitle = NULL,
  text_base_size = 14,
  point_size = 2,
  label_text_size = 4,
  assay.type = NULL,
  ...
)
```

Arguments

`object`	a `SummarizedExperiment` object
`pcs`	numeric vector of length 2, the principal components to plot
`all_features`	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
`center`	logical, should the data be centered prior to PCA? (usually yes)
`scale`	scaling used, as in `prep`. Default is "uv" for unit variance
`n_features`	numeric vector of length two, number of top feature to plot for each principal component
`title, subtitle`	the titles of the plot
`text_base_size`	numeric, base size for text
`point_size`	numeric, size of the points
`label_text_size`	numeric, size of the labels
`assay.type`	character, assay to be used in case of multiple assays
`...`	additional arguments passed to `prep`

Value

A ggplot object.

See Also

pca

Examples

```
data(toy_notame_set, package = "notame")
plot_pca_loadings(toy_notame_set, n_features = c(2, 4))
```

---

plot_p_histogram *Histogram of p-values*

Description

Draws histograms of p-values with expected uniform distribution represented by a dashed red line.

Usage

```
plot_p_histogram(p_values, hline = TRUE, combine = TRUE, x_label = "p-value")
```

Arguments

p_values	list or data frame, each element/column is a vector of p- values. The list names are used as plot titles
hline	logical, whether a horizontal line representing uniform distribution should be plotted
combine	logical, whether plots of individual p-value vectors should be combined into a single object. Set to FALSE if you want to add other plots to the list before plotting
x_label	the x-axis label

Value

If combine = TRUE, a ggplot object. Otherwise a list of ggplot objects.

Examples

```
data(toy_notame_set, package = "notame")
lm_sample <- notameStats::perform_lm(notame::drop_qcs(toy_notame_set),
  "Feature ~ Injection_order")
p_values <- list("Biological samples" = lm_sample$Injection_order.p.value)
plot_p_histogram(p_values)
```

plot_quality *Plot quality metrics*

Description

Plots distribution of each quality metric, and a distribution of the flags.

Usage

```
plot_quality(
  object,
  all_features = FALSE,
  plot_flags = TRUE,
  assay.type = NULL
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
plot_flags	logical, should the distribution of flags be added as a barplot?
assay.type	character, assay to be used in case of multiple assays and no quality metrics are present in feature data

Value

A ggplot object.

Examples

```
data(toy_notame_set, package = "notame")
plot_quality(toy_notame_set)
```

plot_sample_boxplots *Plot a boxplot for each sample*

Description

Plots a boxplot of the distribution of the metabolite values for each sample. The boxplots can be ordered and filled by any combination of columns in the pheno data. By default, order and fill are both determined by the combination of group and time columns.

Usage

```
plot_sample_boxplots(
  object,
  all_features = FALSE,
  order_by,
  fill_by,
  title = "Boxplot of samples",
  subtitle = NULL,
  fill_scale = getOption("notame.fill_scale_dis"),
  zoom_boxplot = TRUE,
  assay.type = NULL
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
order_by	character vector, names of columns used to order the samples
fill_by	character vector, names of columns used to fill the boxplots
title, subtitle	character, title and subtitle of the plot
fill_scale	a scale for the fill of the boxplots, as returned by a ggplot function
zoom_boxplot	logical, whether outliers should be left outside the plot and only the boxplots shown. Defaults to TRUE.
assay.type	character, assay to be used in case of multiple assays

Value

A ggplot object.

Examples

```
data(toy_notame_set, package = "notame")
plot_sample_boxplots(toy_notame_set, order_by = "Group", fill_by = "Group")
```

---

plot_sample_heatmap *Sample heatmap*

Description

Draws a heatmap of the distances between the samples of an experiment, the samples are ordered by hierarchical clustering.

Usage

```
plot_sample_heatmap(
  object,
  all_features = FALSE,
  dist_method = "euclidean",
  clust_method = "ward.D2",
  center = TRUE,
  scale = "uv",
  group_bar = TRUE,
  group = NULL,
  title = "Heatmap of distances between samples",
  subtitle = NULL,
  fill_scale_con = getOption("notame.fill_scale_con"),
  fill_scale_dis = getOption("notame.fill_scale_dis"),
  assay.type = NULL
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
dist_method	distance method used in clustering as in dist
clust_method	method used in clustering as in hclust
center	logical, should the data be centered?
scale	scaling used, as in prep. Default is "uv" for unit variance
group_bar	logical, should a bar showing the groups be drawn under the heat map?
group	character, name of the column used for coloring the group bar
title	The plot title
subtitle	The plot subtitle
fill_scale_con	Continuous fill scale for the heatmap as returned by a ggplot function
fill_scale_dis	Discrete fill scale for the group bar as returned by a ggplot function
assay.type	character, assay to be used in case of multiple assays

Value

A ggplot object. If group_bar is TRUE, the plot will consist of multiple parts and is harder to modify.

See Also

dist hclust

Examples

```
data(toy_notame_set, package = "notame")
plot_sample_heatmap(toy_notame_set, group = "Group")
```

plot_tsne *t-SNE scatter plot*

Description

Computes t-SNE into two dimensions and plots the map points. In case there are missing values, PCA is performed using the nipals method of pca, the method can be changed to "ppca" if nipals fails.

Usage

```
plot_tsne(
  object,
  all_features = FALSE,
  center = TRUE,
  scale = "uv",
  perplexity = 30,
  pca_method = "nipals",
  color = NULL,
  shape = color,
  label = NULL,
  density = FALSE,
  title = "t-SNE",
  subtitle = paste("Perplexity:", perplexity),
  color_scale = NA,
  shape_scale = getOption("notame.shape_scale"),
  fill_scale = getOption("notame.fill_scale_dis"),
  text_base_size = 14,
  point_size = 2,
  assay.type = NULL,
  ...
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
center	logical, should the data be centered prior to PCA? (usually yes)
scale	scaling used, as in prep. Default is '"uv" for unit variance
perplexity	the perplexity used in t-SNE
pca_method	the method used in PCA if there are missing values
color	character, name of the column used for coloring the points. Set to NULL for black color.
shape	character, name of the column used for shape. Set to NULL for uniform round shapes.
label	character, name of the column used for point labels
density	logical, whether to include density plots to both axes. The density curves will be split and colored by the 'color' variable.

title, subtitle	the titles of the plot
color_scale	the color scale as returned by a ggplot function. Set to NA to choose the appropriate scale based on the class of the coloring variable.
shape_scale	the shape scale as returned by a ggplot function
fill_scale	the fill scale used for density curves. If a continuous variable is used as color, density curve will be colorless.
text_base_size	numeric, base size for text
point_size	numeric, size of the points
assay.type	character, assay to be used in case of multiple assays
...	additional arguments passed to Rtsne

Value

A ggplot object. If density is TRUE, the plot will consist of multiple parts and is harder to modify.

See Also

Rtsne

Examples

```
data(toy_notame_set, package = "notame")
plot_tsne(toy_notame_set, color = "Time", shape = "Group", perplexity = 10)
```

---

plot_tsne_arrows *t-SNE plot with arrows*

Description

Computes t-SNE into two dimensions and plots changes according to time. All the observations of a single subject are connected by an arrow ending at the last observation. In case there are missing values, PCA is performed using the nipals method of pca, the method can be changed to "ppca" if nipals fails.

Usage

```
plot_tsne_arrows(
  object,
  all_features = FALSE,
  center = TRUE,
  scale = "uv",
  perplexity = 30,
  pca_method = "nipals",
  color,
  time,
  subject,
  alpha = 0.6,
  arrow_style = arrow(),
  title = "t-SNE changes",
```

```
  subtitle = paste("Perplexity:", perplexity),
  color_scale = getOption("notame.color_scale_dis"),
  text_base_size = 14,
  line_width = 0.5,
  assay.type = NULL,
  ...
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
center	logical, should the data be centered prior to PCA? (usually yes)
scale	scaling used, as in prep. Default is "uv" for unit variance
perplexity	the perplexity used in t-SNE
pca_method	the method used in PCA if there are missing values
color	character, name of the column used for coloring the points
time	character, name of the column containing timepoints
subject	character, name of the column containing subject identifiers
alpha	numeric, value for the alpha parameter of the arrows (transparency)
arrow_style	a description of arrow heads, the size and angle can be modified, see ?arrow
title, subtitle	the titles of the plot
color_scale	the color scale as returned by a ggplot function
text_base_size	the base size of the text
line_width	the width of the arrows
assay.type	character, assay to be used in case of multiple assays
...	additional arguments passed to Rtsne

Value

A ggplot object. If density is TRUE, the plot will consist of multiple parts and is harder to modify.

See Also

Rtsne

Examples

```
data(toy_notame_set, package = "notame")
plot_tsne_arrows(notame::drop_qcs(toy_notame_set), perplexity = 10,
  color = "Group", time = "Time", subject = "Subject_ID")
# If the sample size is large, plot groups separately
plot_tsne_arrows(notame::drop_qcs(toy_notame_set), perplexity = 10,
  color = "Group", time = "Time", subject = "Subject_ID") +
    facet_wrap(~Group)
```

`plot_tsne_hexbin` *t-SNE hexbin plot*

Description

Computes t-SNE into two dimensions and plots the map as hexagonal bins, where the value of the coloring variable is summarised for each bin, by default as the mean of the values inside the bin. In case there are missing values, PCA is performed using the nipals method of `pca`, the method can be changed to "ppca" if nipals fails.

Usage

```
plot_tsne_hexbin(
  object,
  all_features = FALSE,
  center = TRUE,
  scale = "uv",
  pca_method = "nipals",
  perplexity = 30,
  fill = "Injection_order",
  summary_fun = "mean",
  bins = 10,
  title = "t-SNE",
  subtitle = paste("Perplexity:", perplexity),
  fill_scale = getOption("notame.fill_scale_con"),
  assay.type = NULL,
  ...
)
```

Arguments

`object`	a SummarizedExperiment object
`all_features`	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
`center`	logical, should the data be centered prior to PCA? (usually yes)
`scale`	scaling used, as in `prep`. Default is "uv" for unit variance
`pca_method`	the method used in PCA if there are missing values
`perplexity`	the perplexity used in t-SNE
`fill`	character, name of the column used for coloring the hexagons
`summary_fun`	the function used to compute the value for each hexagon
`bins`	the number of bins in x and y axes
`title, subtitle`	the titles of the plot
`fill_scale`	the fill scale as returned by a ggplot function
`assay.type`	character, assay to be used in case of multiple assays
`...`	additional arguments passed to `Rtsne`

Value

A ggplot object.

See Also

Rtsne

Examples

```
data(toy_notame_set, package = "notame")
plot_tsne_hexbin(toy_notame_set, perplexity = 10)
```

`save_batch_plots` *Save batch correction plots*

Description

Saves plots of each feature showing the effect of batch correction. Plots show QC samples and regular samples inside each batch, plus the batch mean for biological samples and QC samples as a horizontal line. The dashed line represents QC mean, the filled line represents biological sample mean. NOTE: if you change the shape variable, be sure to set a shape scale as well, the default scale only has 2 values, so it can only accomodate 2 shapes.

Usage

```
save_batch_plots(
  orig,
  corrected,
  file,
  save = TRUE,
  width = 14,
  height = 10,
  batch = "Batch",
  color = "Batch",
  shape = "QC",
  color_scale = getOption("notame.color_scale_dis"),
  shape_scale = scale_shape_manual(values = c(15, 21)),
  assay.type1 = NULL,
  assay.type2 = NULL
)
```

Arguments

`orig, corrected`	SummarizedExperiment objects before and after batch effect correction
`file`	path to the PDF file where the plots will be saved
`save`	logical, if false, the plots are not saved but returned as a list
`width, height`	width and height of the plots in inches
`batch, color, shape`	column names of pheno data for batch labels, and column used for coloring and shaping points (by default batch and QC)

color_scale, shape_scale
: scales for color and scale as returned by ggplot functions.

assay.type1
: character, assay of orig to be used in case of multiple assays.

assay.type2
: character, assay of corrected to be used in case of multiple assays. If corrected is not supplied, this argument selects another assay from orig.

Value

None, the function is invoked for its plot-saving side effect.

Examples

```
data(toy_notame_set, package = "notame")
# Batch correction
batch_corrected <- batchCorr::normalizeBatches(toy_notame_set,
  assay.type = 1, batches = "Batch", sampleGroup = "Group", refGroup = "QC",
  population = "all", name = "normalized")
# Plots of each feature
save_batch_plots(
  orig = toy_notame_set[1:10], corrected = batch_corrected[1:10],
  file = "batch_plots.pdf", assay.type2 = "normalized"
)
```

---

save_beeswarm_plots *Save beeswarm plots of each feature by group*

Description

Draws a beeswarm plot of feature abundances in each group. A separate plot is drawn and saved for each feature.

Usage

```
save_beeswarm_plots(
  object,
  all_features = FALSE,
  save = TRUE,
  file_path = NULL,
  format = "emf",
  x,
  add_boxplots = FALSE,
  title = "Feature_ID",
  subtitle = NULL,
  color,
  color_scale = getOption("notame.color_scale_dis"),
  text_base_size = 14,
  cex = 2,
  size = 2,
  title_line_length = 40,
  theme = theme_bw(base_size = text_base_size),
  assay.type = NULL,
  ...
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
save	logical, if false, the plots are not saved but returned as a list
file_path	character, a file path for PDF or prefix added to the file paths for other formats
format	character, format in which the plots should be saved
x	character, name of the column to be used as x-axis
add_boxplots	logical, should boxplots be added to the figure?
title, subtitle	column names from feature data to use as plot title/filename and subtitle. Set to NULL for no title/subtitle, this creates running numbered filenames
color	character, name of the column to be used for coloring
color_scale	the color scale as returned by a ggplot function
text_base_size	integer, base size for text in figures
cex	numeric, scaling for adjusting point spacing
size	numeric, size of points
title_line_length	integer, maximum length of the title line in characters, passed to str_wrap
theme	a ggplot theme to be added to the plot
assay.type	character, assay to be used in case of multiple assays
...	other arguments to graphic device functions, like width and height

Value

By default, the function is invoked for its plot-saving side effect. The function returns a list of plots when save = FALSE.

See Also

save_plot

Examples

```
data(toy_notame_set, package = "notame")
# Default beeswarms by group
save_beeswarm_plots(notame::drop_qcs(toy_notame_set)[1:10],
  file_path = "./beeswarm_plots.pdf",
  format = "pdf", x = "Group", color = "Group"
)
# x and color can be a different variable
save_beeswarm_plots(notame::drop_qcs(toy_notame_set)[1:10],
  file_path = "./beeswarm_plots/",
  format = "png",
  x = "Time",
  color = "Group"
)

# Plot one feature
save_beeswarm_plots(notame::drop_qcs(toy_notame_set)[1, ], save = FALSE,
```

```
x = "Group", color = "Group")
```

`save_dc_plots` *Save drift correction plots*

Description

Plots the data before and after drift correction, with the regression line drawn with the original data. If the drift correction was done on log-transformed data, then plots of both the original and log-transformed data before and after correction are drawn. The plot shows 2 standard deviation spread for both QC samples and regular samples.

Usage

```
save_dc_plots(
  orig,
  dc,
  file,
  save = TRUE,
  log_transform = TRUE,
  width = 16,
  height = 8,
  color = "QC",
  shape = color,
  color_scale = getOption("notame.color_scale_dis"),
  shape_scale = scale_shape_manual(values = c(15, 16)),
  assay.orig = NULL,
  assay.dc = NULL
)
```

Arguments

`orig`	a SummarizedExperiment object with assay before drift correction
`dc`	a SummarizedExperiment object with assay after drift correction
`file`	path to the PDF file where the plots should be saved
`save`	logical, if false, the plots are not saved but returned as a list
`log_transform`	logical, was the drift correction done on log- transformed data?
`width, height`	width and height of the plots in inches
`color`	character, name of the column used for coloring the points
`shape`	character, name of the column used for shape
`color_scale`	the color scale as returned by a ggplot function
`shape_scale`	the shape scale as returned by a ggplot function
`assay.orig`	character, name of assay with abundances before correction
`assay.dc`	character, name of assay after correction

Details

By default, the column used for color is also used for shape.

Value

None, the function is invoked for its plot-saving side effect.

See Also

correct_drift

Examples

```
data(toy_notame_set, package = "notame")

toy_notame_set <- notame::mark_nas(toy_notame_set, value = 0)
dc <- notame::correct_drift(toy_notame_set, assay.type = 1,
                            name = "corrected")
save_dc_plots(toy_notame_set[1, ], dc[1, ],
  file = "drift_plots.pdf",
  assay.orig = 1, assay.dc = "corrected")
```

---

save_group_boxplots *Save box plots of each feature by group*

Description

Draws a boxplot of feature abundances in each group. A separate plot is drawn and saved for each feature.

Usage

```
save_group_boxplots(
  object,
  all_features = FALSE,
  save = TRUE,
  file_path = NULL,
  format = "emf",
  x,
  color,
  title = "Feature_ID",
  subtitle = NULL,
  color_scale = getOption("notame.color_scale_dis"),
  text_base_size = 14,
  box_width = 0.8,
  line_width = 0.5,
  point_size = 3,
  title_line_length = 40,
  theme = theme_bw(base_size = text_base_size),
  assay.type = NULL,
  ...
)
```

Arguments

object	a SummarizedExperiment object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
save	logical, if false, the plots are not saved but returned as a list
file_path	character, a file path for PDF or prefix added to the file paths for other formats
format	character, format in which the plots should be saved
x	character, name of the column to be used as x-axis
color	character, name of the column to be used for coloring
title, subtitle	column names from feature data to use as plot title/filename and subtitle. Set to NULL for no title/subtitle, this creates running numbered filenames
color_scale	the color scale as returned by a ggplot function
text_base_size	integer, base size for text in figures
box_width	numeric, width of the boxes
line_width	numeric, width of the lines
point_size	numeric, size of the mean points
title_line_length	integer, maximum length of the title line in characters, passed to str_wrap
theme	a ggplot theme to be added to the plot
assay.type	character, assay to be used in case of multiple assays
...	other arguments to graphic device functions, like width and height

Value

By default, the function is invoked for its plot-saving side effect. The function returns a list of plots when save = FALSE.

See Also

save_plot

Examples

```
data(toy_notame_set, package = "notame")
# Default boxplots by group
save_group_boxplots(notame::drop_qcs(toy_notame_set)[1:10],
  file_path = "./group_boxplots.pdf",
  format = "pdf", x = "Group", color = "Group"
)
# x and color can be a different variable
save_group_boxplots(notame::drop_qcs(toy_notame_set)[1:10],
  file_path = "./time_boxplots/",
  format = "emf",
  x = "Time",
  color = "Group"
)
# Plot one feature
save_group_boxplots(notame::drop_qcs(toy_notame_set)[1, ], save = FALSE,
  x = "Group", color = "Group")
```

`save_group_lineplots` *Save line plots with errorbars by group*

Description

Plots the change in the feature abundances as a function of e.g. time. A line is drawn for each group and error bars are added. A separate plot is drawn for each feature.

Usage

```
save_group_lineplots(
  object,
  all_features = FALSE,
  save = TRUE,
  file_path = NULL,
  format = "emf",
  x,
  group,
  title = "Feature_ID",
  subtitle = NULL,
  fun.data = "mean_cl_boot",
  fun = NULL,
  fun.min = NULL,
  fun.max = NULL,
  position_dodge_amount = 0.2,
  color_scale = getOption("notame.color_scale_dis"),
  text_base_size = 14,
  line_width = 0.5,
  point_size = 4,
  title_line_length = 40,
  theme = theme_bw(base_size = text_base_size),
  assay.type = NULL,
  ...
)
```

Arguments

`object`	a `SummarizedExperiment` object
`all_features`	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization
`save`	logical, if false, the plots are not saved but returned as a list
`file_path`	character, a file path for PDF or prefix added to the file paths for other formats
`format`	character, format in which the plots should be saved
`x`	character, name of the column to be used as x-axis
`group`	character, name of the column containing group information, used for coloring
`title, subtitle`	column names from feature data to use as plot title/filename and subtitle. Set to NULL for no title/subtitle, this creates running numbered filenames
`fun.data`	passed to `stat_summary` and used for errorbars, "A function that is given the complete data and should return a data frame with variables ymin, y, and ymax."

`fun.min`, `fun`, `fun.max`
: Alternative to fun.data, passed to `stat_summary`, "supply three individual functions that are each passed a vector of x's and should return a single number"

`position_dodge_amount`
: numeric: how much the group mean points should dodge away from each other

`color_scale`
: the color scale as returned by a ggplot function

`text_base_size`
: integer, base size for text in figures

`line_width`
: numeric, width of the lines

`point_size`
: numeric, size of the points

`title_line_length`
: integer, maximum length of the title line in characters, passed to `str_wrap`

`theme`
: a ggplot theme to be added to the plot

`assay.type`
: character, assay to be used in case of multiple assays

`...`
: other arguments to graphic device functions, like width and height

Value

By default, the function is invoked for its plot-saving side effect. The function returns a list of plots when `save = FALSE`.

See Also

`save_plot`, `stat_summary`

Examples

```
data(toy_notame_set, package = "notame")
save_group_lineplots(notame::drop_qcs(toy_notame_set)[1:10],
  file_path = "./group_line_plots.pdf",
  format = "pdf", x = "Time", group = "Group"
)
save_group_lineplots(notame::drop_qcs(toy_notame_set)[1:10],
  file_path = "./group_line_plots/",
  format = "png", x = "Time", group = "Group"
)
# Plot one feature
save_group_lineplots(notame::drop_qcs(toy_notame_set[1, ]), save = FALSE,
x = "Time", group = "Group")
```

---

save_plot *Save plot to chosen format*

Description

Saves the given plot to a file. Supports pdf, svg, emf, png and tiff formats. If an error occurs with the plot, an empty file is created.

Usage

```
save_plot(p, file, ...)
```

Arguments

p	a ggplot object
file	the file path
...	other arguments to plot function, like width and height

Value

None, the function is invoked for its plot-saving side effect.

See Also

pdf, emf, svg, png, tiff

Examples

```
data(toy_notame_set, package = "notame")

p <- plot_sample_heatmap(toy_notame_set, group = "Group")

save_plot(p, file = "test.pdf")
```

---

save_QC_plots *Write all relevant pretreatment visualizations to pdf*

Description

A wrapper around all the major visualization functions, used for visualizing data between major steps of data preprocessing. Saves all visualizations as PDFs with a set prefix on filenames.

Usage

```
save_QC_plots(
  object,
  prefix,
  format = "pdf",
  perplexity = 30,
  merge = FALSE,
  remove_singles = FALSE,
  group = NULL,
  time = NULL,
  id = NULL,
  color = NULL,
  assay.type = NULL
)
```

Arguments

object	a SummarizedExperiment object
prefix	character, a file path prefix added to the file paths
format	character, format in which the plots should be saved, DOES NOT support raster formats
perplexity	perplexity for t-SNE plots
merge	logical, whether the files should be merged to a single PDF, see Details
remove_singles	logical, whether to remove single plot files after merging. Only used if merge = TRUE
group	character, name of pheno data column containing the group labels
time	character, name of pheno data column containing timepoints
id	character, name of pheno data column containing subject identifiers
color	character, name of pheno data column used for coloring sample labels for dendrograms
assay.type	character, assay to be used in case of multiple assays

Details

If merge is TRUE and format is pdf, then a file containing all the visualizations named prefix.pdf will be created. NOTE: on Windows this requires installation of pdftk (https://www.pdflabs.com/tools/pdftk-the-pdf-toolkit/) and on Linux you need to have pdfunite installed. On MacOS, no external software is needed. Note that at least on Windows, prefix should be a path from the root, so that the underlying system command will find the files. The type of visualizations to be saved depends on the type of object. Here is a comprehensive list of the visualizations:

- Distribution of quality metrics and flags plot_quality
- Boxplots of each sample in injection order plot_sample_boxplots
- PCA scores plot of samples colored by injection order plot_pca
- t-SNE plot of samples colored by injection order plot_tsne
- If the object has over 60 samples, hexbin versions of the PCA and t- SNE plots above plot_pca_hexbin, plot_tsne_hexbin
- Dendrogram of samples ordered by hierarchical clustering, sample labels colored by group if present plot_dendrogram
- heat map of intersample distances, ordered by hierarchical clustering plot_sample_heatmap
- If the object has QC samples:
  - Density function of the intersample distances in both QCs and biological samples plot_dist_density
  - Histograms of p-values from linear regression of features against injection order in both QCs and biological samples plot_p_histogram
- If the object has a group column:
  - PCA and tSNE plots with points shaped and colored by group plot_pca, plot_tsne
- If the object has a time column:
  - PCA and tSNE plots with points shaped and colored by time 'plot_pca, plot_tsne
  - Dendrogram of samples ordered by hierarchical clustering, sample labels colored by time point plot_dendrogram
- If the object has a group column OR a time column:

  - Boxplots of samples ordered and colored by group and/or time plot_sample_boxplots
- If the object has a group column AND a time column:
  - PCA and tSNE plots with points shaped by group and colored by time plot_pca, plot_tsne
- If the object has a time column AND a subject column:
  - PCA and tSNE plots with arrows connecting the samples of each subject in time point order plot_pca_arrows, plot_tsne_arrows

Value

None, the function is invoked for its plot-saving side effect.

See Also

save_plot

Examples

```
data(toy_notame_set, package = "notame")
rp_neg_set <- toy_notame_set[rowData(toy_notame_set)$Split == "RP_neg", ]
save_QC_plots(rp_neg_set, prefix="figures/RP_neg", perplexity=5,
              group = "Group", color = "Group", time = "Time",
              id = "Subject_ID")
```

---

save_scatter_plots *Save scatter plots of each feature against a set variable*

Description

Draws a scatterplots with a feature on y-axis and another variable on x-axis. A separate plot is drawn and saved for each feature.

Usage

```
save_scatter_plots(
  object,
  x = "Injection_order",
  save = TRUE,
  file_path = NULL,
  format = "emf",
  all_features = FALSE,
  color = NULL,
  color_scale = NA,
  shape = NULL,
  title = "Feature_ID",
  subtitle = NULL,
  shape_scale = getOption("notame.shape_scale"),
  text_base_size = 14,
  point_size = 2,
  title_line_length = 40,
```

```
  theme = theme_bw(base_size = text_base_size),
  assay.type = NULL,
  ...
)
```

Arguments

object	a SummarizedExperiment object
x	character, name of the column to be used as x-axis
save	logical, if false, the plots are not saved but returned as a list
file_path	character, a file path for PDF or prefix added to the file paths for other formats
format	character, format in which the plots should be saved
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
color	character, name of the column to be used for coloring
color_scale	the color scale as returned by a ggplot function. Set to NA to choose the appropriate scale based on the class of the coloring variable.
shape	character, name of the column used for shape
title, subtitle	column names from feature data to use as plot title/filename and subtitle. Set to NULL for no title/subtitle, this creates running numbered filenames
shape_scale	the shape scale as returned by a ggplot function
text_base_size	integer, base size for text in figures
point_size	numeric, size of the points
title_line_length	integer, maximum length of the title line in characters, passed to str_wrap
theme	a ggplot theme to be added to the plot
assay.type	character, assay to be used in case of multiple assays
...	other arguments to graphic device functions, like width and height

Value

By default, the function is invoked for its plot-saving side effect. The function returns a list of plots when save = FALSE.

See Also

save_plot

Examples

```
data(toy_notame_set, package = "notame")
# Against injection order, colored by group
save_scatter_plots(
  object = toy_notame_set[1:10],
  x = "Injection_order",
  color = "Group",
  file_path = "./scatter_plots.pdf",
  format = "pdf"
)
```

```
# Plot one feature
save_scatter_plots(toy_notame_set[1, ], save = FALSE)
```

`save_subject_line_plots` *Save line plots with mean*

Description

Plots the change in the feature abundances as a function of e.g. time. A line is drawn for each subject and a mean line is added. A separate plot is drawn and saved for each feature.

Usage

```
save_subject_line_plots(
  object,
  all_features = FALSE,
  save = TRUE,
  file_path = NULL,
  format = "emf",
  x,
  id,
  title = "Feature_ID",
  subtitle = NULL,
  color = NULL,
  color_scale = getOption("notame.color_scale_dis"),
  facet = NULL,
  text_base_size = 14,
  line_width = 0.3,
  mean_line_width = 1.2,
  title_line_length = 40,
  theme = theme_bw(base_size = text_base_size),
  assay.type = NULL,
  ...
)
```

Arguments

`object`	a `SummarizedExperiment` object
`all_features`	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
`save`	logical, if false, the plots are not saved but returned as a list
`file_path`	character, a file path for PDF or prefix added to the file paths for other formats
`format`	character, format in which the plots should be saved
`x`	character, name of the column to be used as x-axis
`id`	character, name of the column containing subject IDs
`title, subtitle`	column names from feature data to use as plot title/filename and subtitle. Set to NULL for no title/subtitle, this creates running numbered filenames

color	character, the column name to color the lines by (optional)
color_scale	the color scale as returned by a ggplot function
facet	character, the column name to facet by (optional, usually same as color)
text_base_size	integer, base size for text in figures
line_width	numeric, width of the lines
mean_line_width	numeric, width of the mean line
title_line_length	integer, maximum length of the title line in characters, passed to str_wrap
theme	a ggplot theme to be added to the plot
assay.type	character, assay to be used in case of multiple assays
...	other arguments to graphic device functions, like width and height

Value

By default, the function is invoked for its plot-saving side effect. The function returns a list of plots when save = FALSE.

See Also

save_plot

Examples

```
data(toy_notame_set, package = "notame")
save_subject_line_plots(notame::drop_qcs(toy_notame_set)[1:10], x = "Time",
  id = "Subject_ID", file_path = "./subject_line_plots.pdf",
  format = "emf", title = NULL)

# Plot one feature
save_subject_line_plots(notame::drop_qcs(toy_notame_set[1, ]), save = FALSE,
  x = "Time", id = "Subject_ID")
```

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visualize_clusters *Visualize clusters of features*

Description

Draws multiple visualizations of each cluster, creating a separate file for each cluster.

Usage

```
visualize_clusters(
  object,
  min_size = 3,
  rt_window = 1/60,
  n_clust_col = "Cluster_size",
  clust_col = "Cluster_features",
```

```
  mpa_col = "MPA",
  mz_col = NULL,
  rt_col = NULL
)
```

Arguments

object	a SummarizedExperiment object with clustering metadata
min_size	the minimum number of features a cluster needs to have to be plotted
rt_window	numeric, the retention time window to use in linking features. NOTE you need to use the same unit as in the retention time column
n_clust_col	character, name of the column that contains the features included in cluster, separated by semicolon
clust_col	character, name of the column that contains the features in a cluster
mpa_col	character, name of column that contains median peak area of features
mz_col	character, name of the column in features that contains mass-to-charge ratios
rt_col	character, name of the column in features that contains retention times

Details

Note that the input data has been assigned clusters but has not yet been compressed, for example by retaining the feature with the highest median peak area.

Value

A list with clusters containing two plots, a heatmap

Examples

```
data(toy_notame_set, package = "notame")
# The parameters are really weird because example data is imaginary
clustered <- notame::cluster_features(toy_notame_set, rt_window = 1,
                                      corr_thresh = 0.5, d_thresh = 0.6)

cluster_plots <- visualize_clusters(clustered, rt_window = 1)
```

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volcano_plot *Volcano plot*

Description

Draws a volcano plot of effect size and p-values.

Usage

```
volcano_plot(
  object,
  x,
  p,
  p_fdr = NULL,
  color = NULL,
  p_breaks = c(0.05, 0.01, 0.001, 1e-04),
  fdr_limit = 0.05,
  log2_x = FALSE,
  center_x_axis = TRUE,
  x_lim = NULL,
  label = NULL,
  label_limit = 0.05,
  color_scale = getOption("notame.color_scale_con"),
  title = "Volcano plot",
  subtitle = NULL,
  text_base_size = 14,
  label_text_size = 4,
  ...
)
```

Arguments

object	a SummarizedExperiment object or a data frame. Feature data is used. If x is a data frame, it is used as is.
x, p	the column names of effect size (x-axis) and p-values
p_fdr	column name of FDR corrected p-values, used to draw a line showing the fdr-corrected significance level
color	column name used to color the plots
p_breaks	a numerical vector of the p_values to show on the y-axis
fdr_limit	the significance level used in the experiment
log2_x	logical, whether effect size should be plotted on a log2 axis.
center_x_axis	logical, whether x-axis should be centered. If TRUE, the "zero-effect" will be on the middle of the plot. The "zero effect" is 0 if log2_x = FALSE and 1 if log2_x = TRUE
x_lim	numerical vector of length 2 for manually setting the x-axis limits
label	column name used to label the plots
label_limit	numeric, p-value which is used to limit label plotting. Defaults to 0.05.
color_scale	the color scale as returned by a ggplot function
title, subtitle	the title and subtitle of the plot
text_base_size	integer, base size for text in figures
label_text_size	numeric, size of the labels
...	parameters passed to geom_point, such as shape and alpha values. New aesthetics can also be passed using mapping = aes(...).

Value

A ggplot object.

Examples

```
data(toy_notame_set, package = "notame")
# naturally, this looks messy as there are not enough p-values
lm_results <- notameStats::perform_lm(notame::drop_qcs(toy_notame_set),
  formula_char = "Feature ~ Group")
volcano_plot(lm_results,
  x = "GroupB.estimate",
  p = "GroupB.p.value", p_fdr = "GroupB.p.value_FDR",
  label = "Feature_ID",
  fdr_limit = 0.1
)
```

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