# Package 'notameViz'

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```
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manhattan_plot	Manhattan plot
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## 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 <code>geom_point</code> , such as shape and alpha values. New aesthetics can also be passed using mapping = aes().

### Value

A ggplot object.

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#### **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),</pre>
  formula_char = "Feature ~ Group")
lm_data <- dplyr::left_join(as.data.frame(rowData(toy_notame_set)),</pre>
  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)</pre>
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**

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.

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<pre>mz_col, rt_col</pre>	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 <code>geom_point</code> , such as shape and alpha values. New aesthetics can also be passed using mapping = <code>aes()</code> .

#### Value

A ggplot object.

#### **Examples**

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",
```

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```
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.

plot\_dist\_density 7

#### 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 logical, should all features be used? If FALSE (the default), flagged features are all\_features removed before visualization. dist\_method method for calculating the distances, passed to dist center logical, should the data be centered? scaling used, as in prep Default is "uv" for unit variance scale color\_scale a scale for the color of the edge of density curves, as returned by a ggplot funcfill\_scale a scale for the fill of the density curves, as returned by a ggplot function title the plot title the plot subtitle subtitle

character, assay to be used in case of multiple assays

### Value

A ggplot object.

assay.type

### See Also

dist

```
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))
```

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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,
  х,
  у,
  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.)	

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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. if discretize\_effect = TRUE, either the number of breaks or the points where breaks 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? logical, if clustering = FALSE, lower\_tri = FALSE, should the order of the reverse\_y 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

#### **Details**

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

the appropriate scale based on the class of the effect variable.

fill scale for the heatmap as returned by a ggplot function. Set to NA to choose

#### Value

A ggplot object.

fill scale

title, subtitle the title and subtitle of the plot

### See Also

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

```
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",</pre>
```

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```
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.

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### 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
<pre>point_size</pre>	numeric, size of the points
assay.type	character, assay to be used in case of multiple assays
	additional arguments passed to pca

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#### 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)

plot\_pca\_hexbin 13

scaling used, as in prep. Default is "uv" for unit variance scale character, name of the column used for coloring the arrows color character, name of the column containing timepoints time subject character, name of the column containing subject identifiers numeric, value for the alpha parameter of the arrows (transparency) alpha 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 character, assay to be used in case of multiple assays assay.type additional arguments passed to pca

#### Value

A ggplot object.

#### See Also

рса

## Examples

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.

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#### 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

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

plot\_pca\_loadings 15

### **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
                  numeric vector of length 2, the principal components to plot
pcs
                  logical, should all features be used? If FALSE (the default), flagged features are
all_features
                  removed before visualization.
                  logical, should the data be centered prior to PCA? (usually yes)
center
                  scaling used, as in prep. Default is "uv" for unit variance
scale
                  numeric vector of length two, number of top feature to plot for each principal
n_features
                  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
                  character, assay to be used in case of multiple assays
assay.type
                  additional arguments passed to prep
. . .
```

#### Value

A ggplot object.

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#### 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	
p_varues	inst of data frame, each element/column is a vector of p-values. The fist 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.

```
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)</pre>
```

plot\_quality 17

### **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?

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)
```

### **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.

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#### 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
```

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

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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.

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```
title, subtitle the titles of the plot
color_scale
                   the color scale as returned by a ggplot function. Set to NA to choose the appro-
                   priate scale based on the class of the coloring variable.
                   the shape scale as returned by a ggplot function
shape_scale
                   the fill scale used for density curves. If a continuous variable is used as color,
fill_scale
                   density curve will be colorless.
text_base_size numeric, base size for text
                   numeric, size of the points
point_size
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",
```

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```
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. logical, should the data be centered prior to PCA? (usually yes) center scale scaling used, as in prep. Default is "uv" for unit variance the perplexity used in t-SNE perplexity pca\_method the method used in PCA if there are missing values color character, name of the column used for coloring the points character, name of the column containing timepoints time 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 the width of the arrows

line\_width

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

```
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)
```

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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

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#### 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 accommodate 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)

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```
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"
)</pre>
```

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",
  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
```

```
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,
```

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```
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

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#### **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**

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",
  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,
)
```

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#### **Arguments**

object a SummarizedExperiment object logical, should all features be used? If FALSE (the default), flagged features are all\_features removed before visualization. logical, if false, the plots are not saved but returned as a list save 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 character, name of the column to be used as x-axis Х 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 a ggplot theme to be added to the plot theme character, assay to be used in case of multiple assays assay.type 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
```

```
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")
```

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```
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",
  х,
  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."

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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.

save\_QC\_plots

#### Usage

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

### **Arguments**

```
p a ggplot objectfile 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")</pre>
```

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
```

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#### **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 for t-SNE plots perplexity merge logical, whether the files should be merged to a single PDF, see Details logical, whether to remove single plot files after merging. Only used if merge = remove\_singles **TRUE** group character, name of pheno data column containing the group labels character, name of pheno data column containing timepoints time id character, name of pheno data column containing subject identifiers

color character, name of pheno data column used for coloring sample labels for den-

drograms

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:

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- 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**

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,
```

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

## Arguments

object	a SummarizedExperiment object
Х	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_leng	yth
	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
```

```
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",
 х,
  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
                   logical, should all features be used? If FALSE (the default), flagged features are
all_features
                   removed before visualization.
                   logical, if false, the plots are not saved but returned as a list
save
                   character, a file path for PDF or prefix added to the file paths for other formats
file_path
format
                   character, format in which the plots should be saved
                   character, name of the column to be used as x-axis
х
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
```

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```
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
                   numeric, width of the lines
line_width
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
                   character, assay to be used in case of multiple assays
assay.type
                   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")
```

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",
```

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```
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**

volcano\_plot Volcano plot

## Description

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

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### Usage

```
volcano_plot(
  object,
  Х,
  р,
  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	e
	numeric, size of the labels
	parameters passed to <pre>geom_point</pre> , such as shape and alpha values. New aesthetics can also be passed using mapping = aes().

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### Value

A ggplot object.

```
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
)</pre>
```

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