

# Package ‘notameViz’

June 5, 2026

**Type** Package

**Title** Workflow for non-targeted LC-MS metabolic profiling

**Version** 1.3.0

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

**License** MIT + file LICENSE

**Encoding** UTF-8

**biocViews** BiomedicalInformatics, Metabolomics, DataImport, MassSpectrometry, BatchEffect, MultipleComparison, Normalization, QualityControl, Visualization, Preprocessing

**Depends** R (>= 4.5.0), ggplot2, SummarizedExperiment

**Imports** BiocGenerics, cowplot, devEMF, dplyr, ggbeeswarm, ggdendro, ggrepel, grDevices, limma, methods, notame, pcaMethods, qpdf, Rtsne, scales, stringr, stats, tibble, tidyr, utils

**Suggests** batchCorr, BiocStyle, igraph, knitr, notameStats, testthat

**URL** <https://github.com/hanhineva-lab/notameViz>

**BugReports** <https://github.com/hanhineva-lab/notameViz/issues>

**RoxygenNote** 7.3.3

**VignetteBuilder** knitr

**Config/testthat/parallel** true

**git\_url** <https://git.bioconductor.org/packages/notameViz>

**git\_branch** devel

**git\_last\_commit** bd31848

**git\_last\_commit\_date** 2026-04-28

**Repository** Bioconductor 3.24

**Date/Publication** 2026-06-04

**Author** Anton Klåvus [aut, cph] (ORCID:  
<<https://orcid.org/0000-0003-2612-0230>>),  
Jussi Paananen [aut, cph] (ORCID:  
<<https://orcid.org/0000-0001-5100-4907>>),  
Oskari Timonen [aut, cph] (ORCID:  
<<https://orcid.org/0000-0002-6317-6260>>),

Atte Lihtamo [aut],  
 Vilhelm Suksi [aut, cre] (ORCID:  
<https://orcid.org/0009-0005-1108-518X>),  
 Retu Haikonen [aut] (ORCID: <https://orcid.org/0000-0003-0830-3850>),  
 Leo Lahti [aut] (ORCID: <https://orcid.org/0000-0001-5537-637X>),  
 Kati Hanhineva [aut] (ORCID: <https://orcid.org/0000-0001-6834-7375>),  
 Ville Koistinen [ctb] (ORCID: <https://orcid.org/0000-0003-1587-8361>),  
 Olli Kärkkäinen [ctb] (ORCID: <https://orcid.org/0000-0003-0825-4956>),  
 Artur Sannikov [ctb]

**Maintainer** Vilhelm Suksi <vksuks@utu.fi>

## Contents

manhattan_plot . . . . .	3
mz_rt_plot . . . . .	4
plot_dendrogram . . . . .	5
plot_dist_density . . . . .	6
plot_effect_heatmap . . . . .	8
plot_injection_lm . . . . .	10
plot_pca . . . . .	11
plot_pca_arrows . . . . .	12
plot_pca_hexbin . . . . .	14
plot_pca_loadings . . . . .	15
plot_p_histogram . . . . .	16
plot_quality . . . . .	17
plot_sample_boxplots . . . . .	17
plot_sample_heatmap . . . . .	18
plot_tsne . . . . .	20
plot_tsne_arrows . . . . .	21
plot_tsne_hexbin . . . . .	23
save_batch_plots . . . . .	24
save_beeswarm_plots . . . . .	25
save_dc_plots . . . . .	27
save_group_boxplots . . . . .	28
save_group_lineplots . . . . .	30
save_plot . . . . .	31
save_QC_plots . . . . .	32
save_scatter_plots . . . . .	34
save_subject_line_plots . . . . .	36
visualize_clusters . . . . .	37
volcano_plot . . . . .	38

**Index**

**41**

---

manhattan_plot	<i>Manhattan plot</i>
----------------	-----------------------

---

### 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  $-\log_{10}(\text{p-value})$  on the y-axis will be multiplied by the direction (sign) of the effect, so part of the points will "drop" from the  $p = 1$  ( $-\log_{10}(p) = 0$ ) 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 <a href="#">SummarizedExperiment</a> 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 <a href="#">geom_point</a> , such as shape and alpha values. New aesthetics can also be passed using <code>mapping = aes(...)</code> .

### 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 <a href="#">SummarizedExperiment</a> 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 <code>geom_point</code> , such as shape and alpha values. New aesthetics can also be passed using <code>mapping = aes(...)</code> .

**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	<i>Sample dendrogram</i>
-----------------	--------------------------

---

**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 <a href="#">SummarizedExperiment</a> 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 <a href="#">dist</a>
clust_method	method used in clustering as in <a href="#">hclust</a>
center	logical, should the data be centered?
scale	scaling used, as in <a href="#">prep</a> . 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	<i>Plot distance density</i>
-------------------	------------------------------

---

### 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 <a href="#">SummarizedExperiment</a> 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 <a href="#">dist</a>
center	logical, should the data be centered?
scale	scaling used, as in <a href="#">prep</a> 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

<code>data</code>	a data frame with x and y variables and the effect
<code>x, y</code>	the column names of data with the x and y variables
<code>effect</code>	the column name of the effect, e.g. correlation
<code>p</code>	optional, the column name with p-values. If provided, points that scale by p-value are drawn on top of the heatmap tiles
<code>p_limit</code>	numeric, only p-values below the limit are plotted as points
<code>point_size_range</code>	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
<code>log2_effect</code>	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 <code>discretize_effect = TRUE</code> , either the number of breaks or the points where to cut for the levels, see <a href="#">cut</a>
clustering	logical, whether the order of rows and columns should be ordered by hierarchical clustering?
dist_method	distance method used in clustering, see <a href="#">dist</a>
clust_method	clustering method used in clustering, see <a href="#">hclust</a>
lower_tri	logical, should only the lower triangular be plotted?
reverse_y	logical, if <code>clustering = FALSE</code> , <code>lower_tri = FALSE</code> , 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 <a href="#">coord_fixed</a>
symmetric_aspect_ratio	logical, should the plot panel be a square? If yes, uses <code>ggplot2::theme(aspect.ratio = 1)</code> .
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. High amount of significant p-values indicates a strong drift effect.

### Usage

```

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

```

### Arguments

object	a <a href="#">SummarizedExperiment</a> object
all_features	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
eBayes	logical, whether to use limma's eBayes function to compute p-values. If FALSE (default), ordinary t-statistics are used.
assay.type	character, assay to be used in case of multiple assays.
...	additional arguments passed to <a href="#">eBayes</a> function if eBayes = TRUE

### Value

A ggplot object.

### See Also

[plot\\_p\\_histogram](#) [eBayes](#)

### Examples

```

data(toy_notame_set, package = "notame")
plot_injection_lm(toy_notame_set)
# Use eBayes to get more stable p-values with small sample size
plot_injection_lm(toy_notame_set, eBayes = TRUE)

```

---

`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

<code>object</code>	a <a href="#">SummarizedExperiment</a> object
<code>pcs</code>	numeric vector of length 2, the principal components to plot
<code>all_features</code>	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
<code>center</code>	logical, should the data be centered prior to PCA? (usually yes)
<code>scale</code>	scaling used, as in <a href="#">prep</a> . Default is "uv" for unit variance
<code>color</code>	character, name of the column used for coloring the points. Set to NULL for black color.
<code>shape</code>	character, name of the column used for shape. Set to NULL for uniform round shapes.
<code>label</code>	character, name of the column used for point labels
<code>density</code>	logical, whether to include density plots to both axes. The density curves will be split and colored by the 'color' variable.
<code>title, subtitle</code>	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 <a href="#">pca</a>

**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	<i>PCA plot with arrows</i>
-----------------	-----------------------------

---

**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 <a href="#">SummarizedExperiment</a> 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 <a href="#">prep</a> . 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 <a href="#">?arrow</a>
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 <a href="#">pca</a>

### 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

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

### 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**

<code>object</code>	a <a href="#">SummarizedExperiment</a> object
<code>pcs</code>	numeric vector of length 2, the principal components to plot
<code>all_features</code>	logical, should all features be used? If FALSE (the default), flagged features are removed before visualization.
<code>center</code>	logical, should the data be centered prior to PCA? (usually yes)
<code>scale</code>	scaling used, as in <a href="#">prep</a> . Default is "uv" for unit variance
<code>n_features</code>	numeric vector of length two, number of top feature to plot for each principal component
<code>title, subtitle</code>	the titles of the plot
<code>text_base_size</code>	numeric, base size for text
<code>point_size</code>	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	<i>Plot quality metrics</i>
--------------	-----------------------------

---

### 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 <a href="#">SummarizedExperiment</a> 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	<i>Plot a boxplot for each sample</i>
----------------------	---------------------------------------

---

### 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 <a href="#">SummarizedExperiment</a> 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	<i>Sample heatmap</i>
---------------------	-----------------------

---

**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 <a href="#">SummarizedExperiment</a> 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 <a href="#">dist</a>
clust_method	method used in clustering as in <a href="#">hclust</a>
center	logical, should the data be centered?
scale	scaling used, as in <a href="#">prep</a> . 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 <a href="#">SummarizedExperiment</a> 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 <a href="#">prep</a> . 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 <a href="#">Rtsne</a>

**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	<i>t-SNE plot with arrows</i>
------------------	-------------------------------

---

**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 <a href="#">prep</a> . 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 <a href="#">?arrow</a>
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 <a href="#">Rtsne</a>

### 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 <a href="#">prep</a> . 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 <a href="#">Rtsne</a>

**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	<i>Save batch correction plots</i>
------------------	------------------------------------

---

**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	<a href="#">SummarizedExperiment</a> 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 <a href="#">SummarizedExperiment</a> 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 <a href="#">str_wrap</a>
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 <a href="#">SummarizedExperiment</a> 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 <a href="#">str_wrap</a>
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 <a href="#">SummarizedExperiment</a> 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 <a href="#">stat_summary</a> 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 func-
    tions 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 <a href="#">SummarizedExperiment</a> 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.

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.

### 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	<i>Save scatter plots of each feature against a set variable</i>
--------------------	--

---

### 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 <a href="#">SummarizedExperiment</a> 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 <a href="#">str_wrap</a>
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 <a href="#">SummarizedExperiment</a> 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")
```

---

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 <a href="#">SummarizedExperiment</a> 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)
```

---

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 <a href="#">SummarizedExperiment</a> 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 <a href="#">geom_point</a> , 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  
)
```

# Index

coord\_fixed, [9](#)  
correct\_drift, [28](#)  
cut, [9](#)  
  
dist, [6](#), [7](#), [9](#), [19](#)  
  
eBayes, [10](#)  
emf, [32](#)  
  
geom\_point, [3](#), [5](#), [39](#)  
  
hclust, [6](#), [9](#), [19](#)  
  
manhattan\_plot, [3](#)  
mz\_rt\_plot, [4](#)  
  
pca, [12–16](#), [20](#), [21](#), [23](#)  
pdf, [32](#)  
plot\_dendrogram, [5](#), [33](#)  
plot\_dist\_density, [6](#), [33](#)  
plot\_effect\_heatmap, [8](#)  
plot\_injection\_lm, [10](#)  
plot\_p\_histogram, [10](#), [16](#), [33](#)  
plot\_pca, [11](#), [33](#), [34](#)  
plot\_pca\_arrows, [12](#), [34](#)  
plot\_pca\_hexbin, [14](#), [33](#)  
plot\_pca\_loadings, [15](#)  
plot\_quality, [17](#), [33](#)  
plot\_sample\_boxplots, [17](#), [33](#)  
plot\_sample\_heatmap, [18](#), [33](#)  
plot\_tsne, [20](#), [33](#), [34](#)  
plot\_tsne\_arrows, [21](#), [34](#)  
plot\_tsne\_hexbin, [23](#), [33](#)  
png, [32](#)  
prep, [6](#), [7](#), [11](#), [13–16](#), [19](#), [20](#), [22](#), [23](#)  
  
Rtsne, [21–24](#)  
  
save\_batch\_plots, [24](#)  
save\_beeswarm\_plots, [25](#)  
save\_dc\_plots, [27](#)  
save\_group\_boxplots, [28](#)  
save\_group\_lineplots, [30](#)  
save\_plot, [26](#), [29](#), [31](#), [31](#), [35](#), [37](#)  
save\_QC\_plots, [32](#)  
  
save\_scatter\_plots, [34](#)  
save\_subject\_line\_plots, [36](#)  
stat\_summary, [30](#), [31](#)  
str\_wrap, [26](#), [29](#), [31](#), [35](#), [37](#)  
SummarizedExperiment, [3](#), [4](#), [6](#), [7](#), [10](#), [11](#), [13](#),  
[15](#), [17–20](#), [24](#), [26](#), [29](#), [30](#), [33](#), [35](#), [36](#),  
[38](#), [39](#)  
svg, [32](#)  
  
tiff, [32](#)  
  
visualize\_clusters, [37](#)  
volcano\_plot, [38](#)