

Package ‘AOPfingerprintR’

August 29, 2025

Title Curated Gene Annotation of Adverse Outcome Pathways Related to Human Health

Version 0.0.1

Description The package contains lists of gene identifiers mapped to adverse outcome pathways and their key events as described in <https://doi.org/10.1038/s41597-023-02321-w>. Available gene identifiers are Ensembl, Symbol, and Entrez. Furthermore the package provides functions to enrich Key events and AOPs, performe the AOPfingerprint analysis described in <https://doi.org/10.1002/advs.202203984> and to plot the KE-KE interaction network resulting from KE enrichment analysis.

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Annotate_AOPs	<i>AOP_SSbD_ANNOTATION</i>
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Description

AOP_SSbD_IMPACT_ASSOCIATION

Usage

Annotate_AOPs

Format

A data frame with 6 variables:

AOP AOP ids
SSbD_category SSbD impact category
Endpoint Endpoint
Organ Organ
AOP_name AOP_name
Notes Notes

Source

<https://doi.org/10.1038/s41597-023-02321-w>

aops_new

AOP_KE_GENE_ASSOCIATION_DF

Description

Dataframe of association between AOPs, KEs and ensembl genes

Usage

aops_new

Format

A data frame with 6 variables:

Aop AOP ids
Aop_KE KE ids belonging to Aop id
KE KE id
Annotation GO id mapped to KE
Level Level
Gene Gene id

Source

<https://doi.org/10.1038/s41597-023-02321-w>

aop_ke_table_hure	<i>AOP_KE_ASSOCIATION</i>
-------------------	---------------------------

Description

AOP_KE_MAPPING

Usage

aop_ke_table_hure

Format

A data frame with 5 variables:

Aop AOP ids

Ke KE ids

Ke_type KE type description, possible values are MolecularInitiatingEvent, AdverseOutcome, KeyEvent

Ke_description KE name

a.name AOP name

Source

<https://doi.org/10.1038/s41597-023-02321-w>

aop_names	<i>AOP_NAMES</i>
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Description

AOP_IDS_NAMES_ASSOCIATION

Usage

aop_names

Format

A data frame with 2 variables:

a.AOP_ID AOP ids

a.name AOP names

Source

<https://doi.org/10.1038/s41597-023-02321-w>

Biological_system_annotations
BIOLOGICAL_SYSTEM

Description

BIOLOGICAL_SYSTEM_ANNOTATION

Usage

Biological_system_annotations

Format

A data frame with 11 variables:

a.AOP_ID AOP ids

a.name AOP names

key_event_name Name of the key event in the biological system

ke Key event identifier

level Biological level of organization

system Primary biological system involved

organ_tissue Primary organ or tissue involved

cell Primary cell type involved

cell_component Primary cell component involved

secondary_system Secondary biological system involved, if any

secondary_organ_tissue Secondary organ or tissue involved, if any

secondary_cell Secondary cell type involved, if any

secondary_cell_component Secondary cell component involved, if any

Source

<https://doi.org/10.1038/s41597-023-02321-w>

build_aop_for_aop_fingerprints
Build AOP Enrichment Results for AOP Fingerprints

Description

This function constructs AOP enrichment results for AOP fingerprints based on specified criteria.

Usage

```
build_aop_for_aop_fingerprints(
  aop_enrichment_results,
  ke_enrichment_results,
  min_aop_length = 6,
  percentage_enriched_ke = 0.33
)
```

Arguments

`aop_enrichment_results` Enrichment results for AOPs.

`ke_enrichment_results` Enrichment results for KEs.

`min_aop_length` Minimum length of AOPs. Default is 6.

`percentage_enriched_ke` Percentage of enriched KEs for an AOP to be considered significant. Default is 33%.

`time_var` Variable representing time points.

Value

A list containing two data frames: `detailed_results_only_enriched` and `detailed_results_all_ke_in_aop`.

<code>clust_anno</code>	<i>CLUSTERED_KE</i>
-------------------------	---------------------

Description

KE-cluster associations

Usage

`clust_anno`

Format

A data frame with 3 variables:

`cluster` KE cluster ids

`KEs` KE ids

`Description` KE names

Source

<https://doi.org/10.1038/s41597-023-02321-w>

`compute_the_closest_AOs`*Compute closest adverse outcomes to a given vertex*

Description

This function takes in a vertex (or set of vertices) of interest, an igraph object representing the KE-KE network, a vector of adverse outcomes (AO), and optional parameters threshold and distance, and returns the closest adverse outcomes to the vertex of interest in the KEKE_net. If distance is set to TRUE, it returns both the names of the closest adverse outcomes and the corresponding distances between the vertex of interest and the adverse outcomes.

Usage

```
compute_the_closest_AOs(  
  interesting_vertex,  
  KEKE_net,  
  AO,  
  max_path_length = 10,  
  mode = "out",  
  n_AOs = 20  
)
```

Arguments

<code>interesting_vertex</code>	A string representing the name of the vertex/vertices of interest in the KEKE_net.
<code>KEKE_net</code>	An igraph object representing the knowledge exchange network.
<code>AO</code>	A vector of adverse outcomes.
<code>max_path_length</code>	An integer representing the maximum length of the path allowed to reach an adverse outcome (Including KE and AO).
<code>n_AOs</code>	An integer representing the maximum number adverse outcomes to be added

Value

the function returns a vector of the names of the closest AOs to the vertex of interest in the KEKE_net.

`compute_the_closest_MIEs`*Compute closest molecular initiating events to a given vertex/set of vertices*

Description

This function takes in a vertex (or set of vertices) of interest, an igraph object representing the KE-KE network, a vector of adverse outcomes (AO), and optional parameters threshold and distance, and returns the closest adverse outcomes to the vertex of interest in the KEKE_net. If distance is set to TRUE, it returns both the names of the closest adverse outcomes and the corresponding distances between the vertex of interest and the adverse outcomes.

Usage

```
compute_the_closest_MIEs(
  interesting_vertex,
  KEKE_net,
  MIE,
  max_path_length = 5,
  distance = TRUE,
  mode = "out",
  n_MIEs = 20
)
```

Arguments

interesting_vertex	A string representing the name of the vertex/vertices of interest in the KEKE_net.
KEKE_net	An igraph object representing the knowledge exchange network.
MIE	A character vector representing the list of molecular initiating events (MIEs).
max_path_length	An integer representing the maximum length of the path allowed (Including MIE and KE)
n_MIEs	An integer representing the maximum number adverse outcomes to be added#' @param distance A logical value (TRUE or FALSE) indicating whether to return both the names of the closest adverse outcomes and the corresponding distances (default is FALSE).

Value

the function returns a vector of the names of the closest MIEs to the vertex of interest in the KEKE_net.

convert_enrichment_genes_to_symbols

Convert Gene IDs to Symbols in Enrichment Results

Description

Converts gene identifiers in a data frame of enrichment results to gene symbols. Assumes the genes are stored in a column named Genes as a semicolon-separated string.

Usage

```
convert_enrichment_genes_to_symbols(
  enrichment_df,
  gene_id_type,
  organism,
  genes_human,
  genes_mouse,
  genes_rat
)
```


Arguments

enrichment_df	A data frame with a Genes column containing semicolon-separated gene identifiers.
gene_id_type	A string indicating the type of gene ID used (e.g., "ENSEMBL", "ENTREZID", or "SYMBOL").
organism	A string indicating the organism ("human", "mouse", or "rat").
genes_human	mapping file for human genes
genes_mouse	mapping file for mouse genes
genes_rat	mapping file for rat genes

Value

A data frame with the Genes column converted to gene symbols.

`convert_genes_to_symbol`*Convert a Vector of Gene IDs to Gene Symbols*

Description

Converts a vector of gene identifiers (e.g., ENSEMBL or ENTREZ IDs) to gene symbols for a specified organism. Uses preloaded data frames (genes_human, genes_mouse, genes_rat) from `load_biomaRt_data()`.

Usage

```
convert_genes_to_symbol(  
  genes,  
  gene_id_type,  
  organism,  
  genes_human,  
  genes_mouse,  
  genes_rat  
)
```

Arguments

genes	A character vector of gene identifiers.
gene_id_type	A string indicating the input gene ID type (e.g., "ENSEMBL", "ENTREZID", or "SYMBOL").
organism	A string indicating the organism ("human", "mouse", or "rat").
genes_human	mapping file for human genes
genes_mouse	mapping file for mouse genes
genes_rat	mapping file for rat genes

Value

A character vector of gene symbols.

enrich_KEs_AOPs

*Perform Enrichment Analysis for Key Events***Description**

Conduct enrichment analysis for key events (KEs) using the provided data and parameters.

Usage

```
enrich_KEs_AOPs(
  GList,
  list_gene_sets,
  only_significant = FALSE,
  pval_th = 0.05,
  adj.method = "fdr",
  merge_by = "Ke",
  numerical_properties = "Score",
  background = unique(unlist(list_gene_sets)),
  verbose = TRUE,
  aggregation_function = "median"
)
```

Arguments

GList	A named list of data frames. Each element of the list represents a specific experimental condition. The dataframe must have a column with gene ids named 'Feature', and optional numerical values associated to the genes (e.g. t-test statistics, fold-changes, bmd values, etc)
list_gene_sets	One of the list of gene sets for enrichment analysis provided by the package
only_significant	Logical indicating whether to include only significant results.
pval_th	The p-value threshold for significance.
adj.method	The method for p-value adjustment.
merge_by	The variable for merging the results.
numerical_properties	vector of strings, corresponding to colnames in the dataframes of the GList list that indicates numerical properties of the Features
background	A vector of background genes to compare against.
verbose	boolean if TRUE a txtProgressBar is printed
aggregation_function	Function to be used to aggregate the numerical values of the KEs/AOPs. Possible values are median, mean, min and quantile_05. When using quantile_05 the 5% quantile of the distribution of the values is computed.

Value

A list of enriched key events (KEs) and associated results.

filter_df_no	<i>Filter DataFrame by Column Values</i>
--------------	--

Description

Filters a data frame based on specified columns and filter values.

Usage

```
filter_df_no(mod_stats, filter_column, filter_by)
```

Arguments

mod_stats	A data frame containing model statistics.
filter_column	A character vector specifying the columns to filter.
filter_by	A list of character vectors containing filter values for each column.

Value

Returns a filtered data frame if filtering conditions are met; otherwise, NULL.

geneset_enrichment	<i>Gene Set Enrichment Analysis</i>
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Description

This function performs a gene set enrichment analysis, comparing a list of genes to a reference set across multiple gene sets.

Usage

```
geneset_enrichment(
  genes_of_interest,
  background,
  genesets,
  adj.method = "fdr",
  verbose = FALSE,
  numerical_properties = c("BMD", "BMDU", "BMDL"),
  aggregation_function = "median"
)
```

Arguments

background	A vector of background genes to compare against.
genesets	A named list of gene sets, where each element is a vector of genes belonging to that set.
adj.method	Method for adjusting p-values. Default is "fdr" (False Discovery Rate).
verbose	Logical, indicating whether to print progress messages. Default is FALSE.

numerical_properties

A vector of column names from the genes data frame representing numerical properties to be averaged. Default includes "BMD", "BMDU", and "BMDL".

aggregation_function

Function to be used to aggregate the numerical values of the KEs/AOPs. Possible values are median, mean, min and quantile_05. When using quantile_05 the 5% quantile of the distribution of the values is computed.

genes_human

genes_human

Description

Mapping between ENSEMBL, SYMBOL and ENTREZ human gene IDs

Usage

genes_human

Format

A dataframe with columns *ensembl_gene_id*, *hgnc_symbol*, *entrezgene_id* and *description*. From
human = `useMart("ensembl", dataset = "hsapiens_gene_ensembl", host = "https://dec2021.archive.ensembl.org/")`

genes_mouse

genes_mouse

Description

Mapping between ENSEMBL, SYMBOL and ENTREZ mouse gene IDs

Usage

genes_mouse

Format

A dataframe with columns *ensembl_gene_id*, *hgnc_symbol*, *entrezgene_id* and *description*. From
mouse = `useMart("ensembl", dataset = "mmusculus_gene_ensembl", host = "https://dec2021.archive.ensembl.org/")`

genes_rat	<i>genes_rat</i>
-----------	------------------

Description

Mapping between ENSEMBL, SYMBOL and ENTREZ rat gene IDs

Usage

```
genes_rat
```

Format

A dataframe with columns `ensembl_gene_id`, `hgnc_symbol`, `entrezgene_id` and `description`. From `rat = useMart("ensembl", dataset = "rnorvegicus_gene_ensembl", host = "https://dec2021.archive.ensembl.org/")`

group_enriched_ke_by_tissue	<i>Plot KEs average BMD by tissue</i>
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Description

Plot KEs average BMD by tissue

Usage

```
group_enriched_ke_by_tissue(
  ke_enrichment_results,
  filter_experiment = NULL,
  group_by_time = NULL,
  pheno_colnames = c("TermID", "Experiment", "organ_tissue", "BMD", "Ke_description"),
  relevant_tissues = c("liver", "kidney", "blood", "lung", "brain",
    "brain/nervous tissue", "brain/prefrontal cortex/liver")
)
```

Arguments

<code>ke_enrichment_results</code>	A data frame containing the enrichment data.
<code>filter_experiment</code>	a vector of strings of experiment IDs to be plotted. If NULL no filtering is performed
<code>group_by_time</code>	a string for timeid. If NULL all time points are included in the plot. Use NULL also if timepoint is not a variable included in the experimental setup
<code>pheno_colnames</code>	vector of string indicating the variables from KE enrichment results to be considered for plotting,
<code>relevant_tissues</code>	list of tissues to add in the plot.

Value

A grouped bar plot

human_ens_aop	<i>AOP_HUMAN_ENSEMBL_GENES</i>
---------------	--------------------------------

Description

Mapping between AOP ids and human ensembl genes

Usage

human_ens_aop

Format

A list with AOP ids used as indices. Each position contains a vector of human ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_ens_clusters	<i>CLUSTERED_KE_HUMAN_ENSEMBL_GENES</i>
--------------------	---

Description

Mapping between KE ids and human ensembl genes. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

human_ens_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of human ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_ens_ke	<i>KE_HUMAN_ENSEMBL_GENES</i>
--------------	-------------------------------

Description

Mapping between KE ids and human ensembl genes.

Usage

human_ens_ke

Format

A list with KE ids used as indices. Each position contains a vector of human ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_entrez_aop	<i>AOP_HUMAN_ENTREZ_GENES</i>
------------------	-------------------------------

Description

Mapping between AOP ids and human genes symbols

Usage

human_entrez_aop

Format

A list with AOP ids used as indices. Each position contains a vector of human gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_entrez_clusters	<i>CLUSTERED_KE_HUMAN_ENTREZ_GENES</i>
-----------------------	--

Description

Mapping between KE ids and human gene symbols. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

human_entrez_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of human gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_entrez_ke	<i>KE_HUMAN_ENTREZ_GENES</i>
-----------------	------------------------------

Description

Mapping between KE ids and human gene symbols.

Usage

human_entrez_ke

Format

A list with KE ids used as indices. Each position contains a vector of human gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_symbol_aop	<i>AOP_HUMAN_GENE_SYMBOLS</i>
------------------	-------------------------------

Description

Mapping between AOP ids and human genes symbols

Usage

human_symbol_aop

Format

A list with AOP ids used as indices. Each position contains a vector of human gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_symbol_clusters	<i>CLUSTERED_KE_HUMAN_GENE_SYMBOLS</i>
-----------------------	--

Description

Mapping between KE ids and human gene symbols. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

human_symbol_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of human gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

human_symbol_ke

KE_HUMAN_GENE_SYMBOLS

Description

Mapping between KE ids and human gene symbols.

Usage

human_symbol_ke

Format

A list with KE ids used as indices. Each position contains a vector of human gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

KEKE_net

KE_KE_NETWORK

Description

KE-KE network.

Usage

KEKE_net

Format

It is an igraph object, whose nodes are the clustered KEs, and edges represent their connections. Nodes have the attribute 'ke_description' that includes a description of the KEs, while edges have the attribute 'type.r' that specifies the type of connections.

Source

<https://doi.org/10.1038/s41597-023-02321-w>

ke_names	<i>KE_NAMES</i>
----------	-----------------

Description

KE_IDs_NAMES_ASSOCIATION

Usage

```
ke_names
```

Format

A data frame with 2 variables:

Ke Ke ids

Ke_description KE names

Source

<https://doi.org/10.1038/s41597-023-02321-w>

load_biomaRt_data	<i>Load Ensembl Gene Annotation Data from biomaRt</i>
-------------------	---

Description

Loads gene annotation data for human, mouse, and rat from the December 2021 archive of Ensembl using the biomaRt package. This function retrieves Ensembl gene IDs, gene symbols, Entrez IDs, and descriptions for each species. The resulting data frames (genes_human, genes_mouse, genes_rat) are stored in the global environment.

Usage

```
load_biomaRt_data()
```

Value

None. Side effect: creates global variables genes_human, genes_mouse, and genes_rat.

loop_enrichment_v2 *Enrichment Analysis for Multiple Experiment Genes*

Description

This is a wrapper of the function `geneset_enrichment` to performs enrichment analysis for multiple experiments.

Usage

```
loop_enrichment_v2(
  GList,
  list_gene_sets,
  background,
  only_significant = TRUE,
  pval_th = 0.05,
  adj.method = "fdr",
  merge_by = "Ke",
  numerical_properties = c("Score"),
  verbose = TRUE,
  aggregation_function = "median"
)
```

Arguments

<code>GList</code>	A named list of data frames. Each element of the list represents a specific experimental condition. The dataframe must have a column with gene ids, and optional numerical values associated to the genes (e.g. t-test statistics, fold-changes, bmd values, etc)
<code>list_gene_sets</code>	A list of gene sets for enrichment analysis.
<code>background</code>	Background gene set for enrichment analysis.
<code>only_significant</code>	Logical, whether to include only significant results.
<code>pval_th</code>	P-value threshold for significance.
<code>adj.method</code>	Adjustment method for p-values.
<code>merge_by</code>	Column used to merge results with the AOP-KE mapping table. Available options "Ke" or "Aop"
<code>numerical_properties</code>	vector of strings, corresponding to colnames in the dataframes of the GList list that indicates numerical properties of the Features
<code>verbose</code>	boolean if TRUE a <code>txtProgressBar</code> is printed
<code>aggregation_function</code>	Function to be used to aggregate the numerical values of the KEs/AOPs. Possible values are median, mean, min and <code>quantile_05</code> . When using <code>quantile_05</code> the 5% quantile of the distribution of the values is computed.

Value

A data frame containing the enriched results.

make_visNetwork*Create a Visualization Network*

Description

This function generates a visualization network (visNetwork) based on enrichment data and a network structure.

Usage

```
make_visNetwork(  
  detailed_results,  
  experiment,  
  enlarge_ke_selection = TRUE,  
  ke_id,  
  numerical_variables,  
  pval_variable,  
  gene_variable,  
  convert_to_gene_symbols = F,  
  gene_id_type,  
  organism,  
  max_path_length = 20,  
  n_AOs = 10,  
  n_MIEs = 10,  
  mode = "out",  
  genes_human,  
  genes_mouse,  
  genes_rat  
)
```

Arguments

detailed_results

A data frame containing detailed enrichment results. It should include columns corresponding to the experiment name, KE (Key Event) identifiers, KE descriptions, and other relevant numerical variables.

experiment

The name of the experiment for which the network is being created. This should match the experiment name in the detailed_results data frame.

enlarge_ke_selection

Logical, whether to expand the selection of Key Events (KEs) to include the closest Molecular Initiating Events (MIEs) and Adverse Outcomes (AOs). Default is TRUE.

ke_id

The column name in detailed_results that corresponds to the Key Event (KE) identifier.

numerical_variables

A character vector specifying the names of the columns in detailed_results that contain numerical variables to be included in the network nodes.

pval_variable

The name of the column in detailed_results that contains p-values or adjusted p-values associated with the enrichment results.

gene_variable	The name of the column in detailed_results that contains gene identifiers or gene sets associated with the enrichment results.
convert_to_gene_symbols	Logical, whether to convert gene identifiers to gene symbols using organism-specific mapping. Default is FALSE.
gene_id_type	A character string indicating the type of gene identifiers used (e.g., "ENSEMBL", "ENTREZID", or "SYMBOL").
organism	A character string specifying the organism of interest ("human", "mouse", or "rat").
max_path_length	Maximum length of the shortest path to be used to retrieve close MIEs or AOs if enlarge_ke_selection = TRUE. Default is 20.
n_AOs	Number of AOs to add if enlarge_ke_selection = TRUE. Default is 10.
n_MIEs	Number of MIEs to add if enlarge_ke_selection = TRUE. Default is 10.
mode	Parameter passed to the igraph::shortest.paths function if enlarge_ke_selection = TRUE. Options are "all", "out", or "in". Default is "out".
genes_human	mapping file for human genes
genes_mouse	mapping file for mouse genes
genes_rat	mapping file for rat genes

Value

A list containing two elements:

nodes A data frame of nodes representing the selected KEs, including information on the numerical variables, p-values, and associated genes.

edges A data frame of edges representing the connections between the KEs in the network.

mouse_ens_aop	<i>AOP_MOUSE_ENSEMBL_GENES</i>
---------------	--------------------------------

Description

Mapping between AOP ids and mouse ensembl genes

Usage

```
mouse_ens_aop
```

Format

A list with AOP ids used as indices. Each position contains a vector of mouse ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_ens_clusters	<i>CLUSTERED_KE_MOUSE_ENSEMBL_GENES</i>
--------------------	---

Description

Mapping between KE ids and mouse ensembl genes. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

mouse_ens_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of mouse ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_ens_ke	<i>KE_MOUSE_ENSEMBL_GENES</i>
--------------	-------------------------------

Description

Mapping between KE ids and mouse ensembl genes.

Usage

mouse_ens_ke

Format

A list with KE ids used as indices. Each position contains a vector of mouse ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_entrez_aop	<i>AOP_MOUSE_ENTREZ_GENES</i>
------------------	-------------------------------

Description

Mapping between AOP ids and mouse genes symbols

Usage

mouse_entrez_aop

Format

A list with AOP ids used as indices. Each position contains a vector of mouse gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_entrez_clusters	<i>CLUSTERED_KE_MOUSE_ENTREZ_GENES</i>
-----------------------	--

Description

Mapping between KE ids and mouse gene symbols. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

mouse_entrez_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of mouse gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_entrez_ke	<i>KE_MOUSE_ENTREZ_GENES</i>
-----------------	------------------------------

Description

Mapping between KE ids and mouse gene symbols.

Usage

mouse_entrez_ke

Format

A list with KE ids used as indices. Each position contains a vector of mouse gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_symbol_aop	<i>AOP_MOUSE_GENE_SYMBOLS</i>
------------------	-------------------------------

Description

Mapping between AOP ids and mouse genes symbols

Usage

mouse_symbol_aop

Format

A list with AOP ids used as indices. Each position contains a vector of mouse gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_symbol_clusters	<i>CLUSTERED_KE_MOUSE_GENE_SYMBOLS</i>
-----------------------	--

Description

Mapping between KE ids and mouse gene symbols. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

mouse_symbol_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of mouse gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

mouse_symbol_ke	<i>KE_MOUSE_GENE_SYMBOLS</i>
-----------------	------------------------------

Description

Mapping between KE ids and mouse gene symbols.

Usage

mouse_symbol_ke

Format

A list with KE ids used as indices. Each position contains a vector of mouse gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

plot_visNetwork	<i>Plot a Visualization Network</i>
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Description

This function generates a visualization network (visNetwork) based on the nodes and edges derived from enrichment data. It allows for the visual grouping of nodes based on either AOPs (Adverse Outcome Pathways) or SSbD (Safe and Sustainable by Design) impact categories, and highlights key events (KEs) based on their significance.

Usage

```
plot_visNetwork(  
  nodes,  
  edges,  
  numerical_variables,  
  group_by = "aop",  
  color_enriched = "red",  
  color_not_enriched = "gray"  
)
```

Arguments

nodes	A data frame containing nodes representing Key Events (KEs). Each node should include information such as KE identifiers, KE descriptions, p-values, associated genes, and any numerical variables relevant to the analysis.
edges	A data frame containing edges representing the connections between the KEs in the network. Each edge should include information such as the source and target KE IDs.
numerical_variables	A character vector specifying the names of the columns in nodes that contain numerical data to be displayed in the node tooltips.
group_by	A character string indicating how to group the nodes in the network. Accepts either "aop" (default) to group by Adverse Outcome Pathways, or other specified categories such as "ssbd" to group by SSbD impact categories. Other grouping categories can be the colnames of the nodes parameter

Value

A visNetwork object that can be rendered to create an interactive network visualization. The network will color nodes based on their significance and group them according to the specified category.

rat_ens_aop	<i>AOP_RAT_ENSEMBL_GENES</i>
-------------	------------------------------

Description

Mapping between AOP ids and rat ensembl genes

Usage

rat_ens_aop

Format

A list with AOP ids used as indices. Each position contains a vector of rat ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_ens_clusters	<i>CLUSTERED_KE_RAT_ENSEMBL_GENES</i>
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Description

Mapping between KE ids and rat ensembl genes. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

rat_ens_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of rat ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_ens_ke	<i>KE_RAT_ENSEMBL_GENES</i>
------------	-----------------------------

Description

Mapping between KE ids and rat ensembl genes.

Usage

rat_ens_ke

Format

A list with KE ids used as indices. Each position contains a vector of rat ensembl gene ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_entrez_aop	<i>AOP_RAT_ENTREZ_GENES</i>
----------------	-----------------------------

Description

Mapping between AOP ids and rat genes symbols

Usage

rat_entrez_aop

Format

A list with AOP ids used as indices. Each position contains a vector of rat gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_entrez_clusters	<i>CLUSTERED_KE_RAT_ENTREZ_GENES</i>
---------------------	--------------------------------------

Description

Mapping between KE ids and rat gene symbols. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

rat_entrez_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of rat gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_entrez_ke	<i>KE_RAT_ENTREZ_GENES</i>
---------------	----------------------------

Description

Mapping between KE ids and rat gene symbols.

Usage

rat_entrez_ke

Format

A list with KE ids used as indices. Each position contains a vector of rat gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_symbol_aop	<i>AOP_RAT_GENE_SYMBOLS</i>
----------------	-----------------------------

Description

Mapping between AOP ids and rat genes symbols

Usage

rat_symbol_aop

Format

A list with AOP ids used as indices. Each position contains a vector of rat gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_symbol_clusters	<i>CLUSTERED_KE_RAT_GENE_SYMBOLS</i>
---------------------	--------------------------------------

Description

Mapping between KE ids and rat gene symbols. KEs sharing the same set of genes are clustered in a combined id as KE_id1;KE_id2

Usage

rat_symbol_clusters

Format

A list with clustered KE ids used as indices. Each position contains a vector of rat gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

rat_symbol_ke	<i>KE_RAT_GENE_SYMBOLS</i>
---------------	----------------------------

Description

Mapping between KE ids and rat gene symbols.

Usage

```
rat_symbol_ke
```

Format

A list with KE ids used as indices. Each position contains a vector of rat gene symbol ids

Source

<https://doi.org/10.1038/s41597-023-02321-w>

render_aop_fingerprint_bubble_plot	<i>Render AOP Fingerprint Bubble Plot</i>
------------------------------------	---

Description

This function generates a bubble plot for rendering AOP fingerprint data.

Usage

```
render_aop_fingerprint_bubble_plot(
  enrichment_data,
  group_AOPs = "SSbD_category",
  group_by,
  group_by2,
  x_axis_var,
  y_axis_var = "TermID",
  filter_column,
  filter_by,
  is_group_by_numeric,
  threshold_proportion,
  text_cex = 12
)
```


Arguments

<code>enrichment_data</code>	A data frame containing the enrichment data.
<code>group_by</code>	Variable used for grouping the data.
<code>group_by2</code>	Second variable used for subgrouping the data.
<code>filter_column</code>	Column for filtering the data.
<code>filter_by</code>	Value for filtering the data.
<code>is_group_by_numeric</code>	Logical, whether the grouping variable is numeric.
<code>threshold_proportion</code>	Proportion threshold for filtering data.
<code>text_cex</code>	Text size for labels.
<code>time_var</code>	Column name of timepoint variable

Value

A bubble plot visualizing AOP fingerprint data.

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