

# Package ‘TraianProt’

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**Title** TraianProt: a user-friendly R package for wide format proteomics data downstream analysis

**Version** 0.99.16

**Description** A proteomics data analysis platform that enables the analysis of both label-free and labeled data from Data-Dependent or Data-Independent Acquisition mass spectrometry mode, supporting MaxQuant, MSFragger, DIA-NN, ProteoScape, and Proteome Discoverer output formats. TraianProt provides a comprehensive suite of stepwise downstream analysis modules, which includes data filtering, normalization procedures, and missing value imputation strategies. The platform also incorporates robust statistical frameworks for differential expression testing, with peptide-spectrum match level correction, thereby enhancing the reliability of biological interpretations.

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|              |                                         |
|--------------|-----------------------------------------|
| barplot_func | Create Bar Plot from Enrichment Results |
|--------------|-----------------------------------------|

---

## Description

Generates a bar plot from an `enrichResult` object, faceted by cluster.

## Usage

```
barplot_func(terms, number, conditions, ...)
```

## Arguments

|            |                                                                                                      |
|------------|------------------------------------------------------------------------------------------------------|
| terms      | A list, where the second element ( <code>terms[[2]]</code> ) is an <code>enrichResult</code> object. |
| number     | Numeric. The number of top terms <i>per condition</i> to display.                                    |
| conditions | Character. A title for the plot.                                                                     |
| ...        | Additional arguments passed to <code>enrichplot::barplot</code> .                                    |

## Value

A `ggplot` object.

## Examples

```
# This example requires a valid enrichResult object.
# We will create a minimal synthetic one.
if (requireNamespace("DOSE") && requireNamespace("methods")) {
  dummy_data <- data.frame(
    Cluster = c("Up-regulated", "Down-regulated"),
    Category = "BP", ID = c("GO:0006915", "GO:0007049"),
    Description = c("apoptosis", "cell cycle"),
    p.value = c(0.01, 0.02), adj.P.Val = c(0.01, 0.02),
    query_size = c(50, 40), Count = c(5, 8), term_size = c(100, 120),
    effective_domain_size = 10000, geneID = c("P04637", "P10415"),
    GeneRatio = c("5/50", "8/40"), BgRatio = c("100/10000", "120/10000"),
    Conditions = c("Up-regulated", "Down-regulated")
  )
  dummy_enrich_result <- methods::new("enrichResult", result = dummy_data)
  terms_list <- list(NULL, dummy_enrich_result)
  barplot_func(terms_list, number = 1, conditions = "My Plot")
}
```

---

|                  |                                      |
|------------------|--------------------------------------|
| boxplot_function | Create Boxplot of Sample Intensities |
|------------------|--------------------------------------|

---

### Description

Generates a ggplot2 boxplot of LOG2 intensities, grouped by sample and colored by condition.

### Usage

```
boxplot_function(df, metadata, selected_conditions)
```

### Arguments

|                     |                                                                                              |
|---------------------|----------------------------------------------------------------------------------------------|
| df                  | A data frame containing the LOG2 intensity data.                                             |
| metadata            | A metadata data frame. Must contain 'group' and 'log2_col' columns to map samples to groups. |
| selected_conditions | A character vector of length 2 specifying the two conditions to compare.                     |

### Value

A ggplot object.

### Examples

```
# Create synthetic data
log_df <- data.frame(
  LOG2.C1 = rnorm(20, 10),
  LOG2.C2 = rnorm(20, 10.1),
  LOG2.T1 = rnorm(20, 12),
  LOG2.T2 = rnorm(20, 12.1)
)

meta <- data.frame(
  group = c("Control", "Control", "Treatment", "Treatment"),
  log2_col = c("LOG2.C1", "LOG2.C2", "LOG2.T1", "LOG2.T2")
)

# Generate the boxplot
boxplot_function(log_df, meta, selected_conditions = c("Control", "Treatment"))
```

---

|                               |                                                  |
|-------------------------------|--------------------------------------------------|
| collapse_technical_replicates | Collapse Technical Replicates in Proteomics Data |
|-------------------------------|--------------------------------------------------|

---

### Description

This function identifies technical replicates based on a biological replicate metadata column and collapses them by calculating the mean intensity. It updates both the expression data and the associated metadata.

**Usage**

```
collapse_technical_replicates(df, metadata)
```

**Arguments**

|          |                                                                                                                  |
|----------|------------------------------------------------------------------------------------------------------------------|
| df       | A data.frame or matrix where rows are proteins/features and columns are samples (intensities).                   |
| metadata | A data.frame containing at least two columns: log2_col (matching colnames in df) and bioreplicate (grouping ID). |

**Details**

The function assumes that technical replicates share the same sample\_name ID in the metadata. It cleans the column names by removing trailing numeric indices (e.g., "Sample, 1" becomes "Sample") using regex. If only one technical replicate exists for a biological group, it simply renames the column.

**Value**

A list with two elements:

- data: A data.frame with collapsed biological replicates as columns.
- metadata: A data.frame with one row per biological replicate, updated to match the new column names.

**Examples**

```
# Example metadata
meta <- data.frame(
  log2_col = c("S1, 1", "S1, 2", "S2, 1"),
  sample_name = c("Bio1", "Bio1", "Bio2"),
  intensity_sample_name = c("S1, 1", "S1, 2", "S2, 1"),
  stringsAsFactors = FALSE
)
# Example data
dat <- data.frame(
  `S1, 1` = c(1, 2), `S1, 2` = c(1.2, 2.2), `S2, 1` = c(5, 6),
  check.names = FALSE
)
result <- collapse_technical_replicates(dat, meta)
```

---

corrplot\_function

*Correlation Matrix*


---

**Description**

Calculates a Pearson correlation matrix from a data frame and visualizes it as a tile-based heatmap using ggplot2, overlaying the correlation coefficients.

**Usage**

```
corrplot_function(
  df,
  metadata,
  display = "circle",
  tl.col = "black",
  addCoef.col = "black"
)
```

**Arguments**

|             |                                                                                                                                                                          |
|-------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df          | A data frame. The columns for which correlations are desired should be numeric. Non-numeric columns will be ignored by <code>cor()</code> .                              |
| metadata    | A metadata data frame. Must contain 'group' and 'log2_col' columns to map samples to groups.                                                                             |
| display     | A string specifying the visual representation (e.g., "circle"). <b>Note:</b> This parameter is currently not implemented in the function body, which defaults to 'tile'. |
| tl.col      | A string for text label color (i.e., the variable names). <b>Note:</b> This parameter is currently not implemented in the function body.                                 |
| addCoef.col | A string specifying the color for the overlaid correlation coefficients (e.g., "black").                                                                                 |

**Details**

Generate a ggplot2 Correlation Matrix Heatmap

The function first calculates the correlation matrix using `cor()` with `use = "complete.obs"`, which handles missing values by pairwise deletion. It then melts the matrix into a "long" format suitable for ggplot2. The plot uses `scale_fill_gradient2` to create a divergent color scale (Red -> White -> Blue) centered at 0. `coord_fixed()` ensures square tiles.

**Value**

A ggplot object representing the correlation heatmap.

**Examples**

```
df_sample <- data.frame(
  LOG2.C1 = rnorm(20, mean = 10),
  LOG2.C2 = rnorm(20, mean = 10),
  LOG2.T1 = rnorm(20, mean = 12),
  LOG2.T2 = rnorm(20, mean = 12)
)

meta <- data.frame(
  group = c("Control", "Control", "Treatment", "Treatment"),
  log2_col = c("LOG2.C1", "LOG2.C2", "LOG2.T1", "LOG2.T2")
)

# 2. Generate the plot
p <- corrplot_function(df_sample, meta, addCoef.col = "blue")

# 3. Display the plot (Important: in examples we just call the object)
p
```

**Description**

Creates a boxplot with jittered points for a single protein, comparing two conditions.

**Usage**

```
Diferential_boxplot(
  df,
  metadata,
  protein = NULL,
  LOG2.names,
  selected_conditions
)
```

**Arguments**

|                     |                                                                                              |
|---------------------|----------------------------------------------------------------------------------------------|
| df                  | A data frame with expression data. Must have a 'Protein' column and LOG2 intensity columns.  |
| metadata            | A data frame with sample metadata. Must have 'group' and 'log2_col' columns.                 |
| protein             | A character string specifying the single protein (from the 'Protein' column) to plot.        |
| LOG2.names          | A character vector of all LOG2 sample column names to use.                                   |
| selected_conditions | A character vector of length 2 specifying the two groups from the 'group' column to compare. |

**Value**

This function is called for its side effect of printing a ggplot. It invisibly returns the ggplot object p.

**Examples**

```
# Create synthetic data
df_box <- data.frame(
  Protein = "Prot1",
  LOG2.C1 = rnorm(1, 8), LOG2.C2 = rnorm(1, 8),
  LOG2.T1 = rnorm(1, 9), LOG2.T2 = rnorm(1, 9)
)
metadata_box <- data.frame(
  log2_col = c("LOG2.C1", "LOG2.C2", "LOG2.T1", "LOG2.T2"),
  group = c("Control", "Control", "Treatment", "Treatment")
)
log_names <- c("LOG2.C1", "LOG2.C2", "LOG2.T1", "LOG2.T2")
selected_cond <- c("Treatment", "Control")

# Generate the plot
if (requireNamespace("DOSE")) {
  Diferential_boxplot(df_box, metadata_box, "Prot1", log_names, selected_cond)
}
```

---

|              |                                         |
|--------------|-----------------------------------------|
| dotplot_func | Create Dot Plot from Enrichment Results |
|--------------|-----------------------------------------|

---

## Description

Generates a dot plot from a `compareClusterResult` object, faceted by condition.

## Usage

```
dotplot_func(terms, ...)
```

## Arguments

|       |                                                                                                            |
|-------|------------------------------------------------------------------------------------------------------------|
| terms | A list, where the first element ( <code>terms[[1]]</code> ) is a <code>compareClusterResult</code> object. |
| ...   | Additional arguments passed to <code>enrichplot::dotplot</code> .                                          |

## Value

A `ggplot` object.

## Examples

```
if (requireNamespace("clusterProfiler", quietly = TRUE)) {
  dummy_data <- data.frame(
    Cluster = "Up-regulated",
    Category = "BP",
    ID = "GO:0006915",
    Description = "apoptosis",
    p.value = 0.01,
    p.adjust = 0.01,
    Count = 5,
    GeneRatio = "5/50",
    BgRatio = "100/10000",
    Conditions = "Up-regulated"
  )

  dummy_cc_result <- methods::new("compareClusterResult",
    compareClusterResult = dummy_data
  )
  dotplot_func(list(dummy_cc_result))
}
```



---

|               |                                        |
|---------------|----------------------------------------|
| filter_valids | <i>Filter proteins by valid values</i> |
|---------------|----------------------------------------|

---

## Description

A helper function to filter a protein expression data frame (e.g., from MaxQuant) based on a minimum number of valid (non-NA, non-zero) values across samples.

## Usage

```
filter_valids(
  df,
  metadata,
  unique_proteins,
  min_prop = NULL,
  at_least_one = FALSE,
  labeltype = 1
)
```

## Arguments

|                 |                                                                                                                                            |
|-----------------|--------------------------------------------------------------------------------------------------------------------------------------------|
| df              | A data frame containing the raw protein expression data.                                                                                   |
| metadata        | A data frame mapping intensity column names to groups.                                                                                     |
| unique_proteins | a list containing unique proteins output from obtain_unique_proteins function .                                                            |
| min_prop        | A numeric threshold for the minimum number of valid values. For example, 2 means a protein must be valid in at least 2 samples to be kept. |
| at_least_one    | Considers whether the condition must be met with both or only one condition.                                                               |
| labeltype       | Type of mass spectrometry experiment.                                                                                                      |

## Value

A list containing the filtered data frame ("filtered") and the LOG2-transformed data frame ("LOG2").

## Examples

```
raw_df <- data.frame(
  Protein = c("P1", "P2", "P3", "P4"),
  LOG2_A1 = c(20, 21, NA, 22),
  LOG2_A2 = c(20, NA, NA, 22),
  LOG2_B1 = c(25, 24, 23, NA),
  LOG2_B2 = c(25, 24, 23, 26)
)
meta_df <- data.frame(
  intensity_sample_name = c("A1", "A2", "B1", "B2"),
  group = c("Control", "Control", "Treatment", "Treatment"),
  log2_col = c("LOG2_A1", "LOG2_A2", "LOG2_B1", "LOG2_B2")
)
unique_list <- list(
  data.frame(Protein = character()),
  data.frame(Protein = character())
)
```

```

)

filtered_data <- filter_valids(
  df = raw_df,
  metadata = meta_df,
  unique_proteins = unique_list,
  min_prop = 0.5,
  at_least_one = FALSE,
  labeltype = 1
)

head(filtered_data)

```

---

gostplot\_func

*Manhattan Plot for Functional Enrichment*


---

### Description

This function is a helper wrapper that extracts the raw gprofiler2 results (the third element) from the output of the Goterms\_finder function to generate a Manhattan plot of enriched terms.

### Usage

```
gostplot_func(terms, ...)
```

### Arguments

|       |                                                          |
|-------|----------------------------------------------------------|
| terms | A list of length 3 generated by Goterms_finder function. |
| ...   | Additional arguments passed to gprofiler2::gostplot      |

### Value

A ggplot or plotly object representing the Manhattan plot of functional enrichment.

### Examples

```
gostplot_func(res)
```

---

Goterms\_finder

*Find GO Terms (gprofiler2)*


---

### Description

Performs Gene Ontology (GO) and pathway enrichment analysis for up- and down-regulated proteins using gprofiler2.

## Usage

```
Goterms_finder(
  df,
  raw,
  target,
  numeric_ns,
  mthreshold,
  filter_na,
  organismo,
  custombg,
  platform,
  ...
)
```

## Arguments

|            |                                                                                                                                           |
|------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| df         | A data frame from statistical analysis (e.g., limma), must have 'expression', 'p.value', 'Protein', and/or 'Protein_description' columns. |
| raw        | A data frame of the "raw" data, used to build the background gene list. Must have 'Protein' or 'Protein_description'.                     |
| target     | Character. The target namespace for gconvert (e.g., "ENSG").                                                                              |
| numeric_ns | Character. Namespace for numeric IDs.                                                                                                     |
| mthreshold | Numeric. g:GOST multi-query significance threshold.                                                                                       |
| filter_na  | Logical. Whether gconvert should filter out NA results.                                                                                   |
| organismo  | Character. The organism name for gprofiler2 (e.g., "hsapiens").                                                                           |
| custombg   | Logical. Whether to use a custom background (from raw).                                                                                   |
| platform   | Numeric. An indicator for the data platform (1, 2, 3, or 4).                                                                              |
| ...        | Additional arguments passed to gprofiler2::gost.                                                                                          |

## Value

A list named go\_structures containing: 1. A compareClusterResult object (for plotting). 2. An enrichResult object (for plotting). 3. The raw gost result object (for gostplot).

## Examples

```
limma_df <- data.frame(
  Protein = c("P04637", "P00533", "P01116"),
  Protein_description = c("TP53", "EGFR", "KRAS"),
  expression = c("Up-regulated", "Up-regulated", "Up-regulated"),
  p.value = c(0.001, 0.002, 0.003)
)

# raw_df is needed for the function structure, even if custombg=FALSE
raw_df <- data.frame(
  Protein = c("P04637", "P00533", "P01116", "P62258"),
  Protein_description = c("TP53", "EGFR", "KRAS", "ACTB")
)

# 2. Run the function with checks
# This example requires an internet connection
```

```

if (requireNamespace("gprofiler2", quietly = TRUE)) {
  try(
    {
      go_res <- Goterms_finder(
        df = limma_df,
        raw = raw_df,
        target = "ENSG",
        numeric_ns = "",
        mthreshold = 0.05,
        filter_na = TRUE,
        organismo = "hsapiens",
        custombg = FALSE,
        platform = 1
      )

      # 3. Safe printing (checks if result exists before printing)
      # We check if go_res exists, is a list, and has the expected slot
      if (!is.null(go_res) &&
          is.list(go_res) &&
          length(go_res) >= 1 &&
          inherits(go_res[[1]], "compareClusterResult")) {
        print(head(as.data.frame(go_res[[1]])))
      }
    },
    silent = TRUE
  )
}

```

---

histogram

*Plot a Histogram*


---

## Description

A simple wrapper to plot a histogram for a specific column in a data frame.

## Usage

```
histogram(df, colname, color, title)
```

## Arguments

|         |                                           |
|---------|-------------------------------------------|
| df      | A data frame.                             |
| colname | The name of the (numeric) column to plot. |
| color   | The color for the histogram.              |
| title   | The main title for the plot.              |

## Value

A histogram plot.

**Examples**

```
my_data <- data.frame(p.value = rnorm(100))
histogram(my_data, "p.value", "lightblue", "P-Value Distribution")
```

---

|                   |                          |
|-------------------|--------------------------|
| identify_proteins | <i>Identify Proteins</i> |
|-------------------|--------------------------|

---

**Description**

Identifies unique and common proteins between two data frames.

**Usage**

```
identify_proteins(raw, metadata, platform, selected_conditions)
```

**Arguments**

|                     |                                                                |
|---------------------|----------------------------------------------------------------|
| raw                 | A data frame containing the raw protein expression data.       |
| metadata            | A data frame mapping intensity column names to groups.         |
| platform            | An indicator (e.g., 1) for the data platform (e.g., MaxQuant). |
| selected_conditions | Conditions compared from you experiment.                       |

**Value**

A list containing three data frames: unique\_df1 (proteins unique to df1), unique\_df2 (proteins unique to df2), and common\_df (proteins common to both).

**Examples**

```
metadata_example <- data.frame(
  intensity_sample_name = c("Log_C1", "Log_C2", "Log_T1", "Log_T2"),
  group = c("Control", "Control", "Treatment", "Treatment")
)

raw_example <- data.frame(
  Protein = c("Prot_A", "Prot_B", "Prot_C", "Prot_D"),
  Log_C1 = c(25.1, 24.2, 0, 22.0),
  Log_C2 = c(25.0, 24.5, 0, 22.2),
  Log_T1 = c(0, 26.1, 23.5, 21.9),
  Log_T2 = c(0, 26.0, 23.8, 22.1)
)

plot_result <- identify_proteins(
  raw = raw_example,
  metadata = metadata_example,
  platform = 1,
  selected_conditions = c("Control", "Treatment")
)

print(plot_result)
```

---

|                 |                                                      |
|-----------------|------------------------------------------------------|
| igraph_analysis | <i>Perform igraph Analysis on STRING Subnetworks</i> |
|-----------------|------------------------------------------------------|

---

## Description

Calculates graph theory measures for up- and down-regulated protein networks.

## Usage

```
igraph_analysis(interactions, taxonid, score)
```

## Arguments

|              |                                                                                                                                                                                                           |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| interactions | A list of data frames (like that returned by <code>interactions_up</code> ) containing mapped STRING IDs. <code>interactions[[1]]</code> = up-regulated, <code>interactions[[2]]</code> = down-regulated. |
| taxonid      | Numeric. The NCBI taxonomy ID for the species (e.g., 9606 for human).                                                                                                                                     |
| score        | Numeric. The minimum required interaction score (0-1000).                                                                                                                                                 |

## Value

A list of two data frames, `Upregulated` and `Downregulated`, containing graph measures for each network.

## Examples

```
if (requireNamespace("STRINGdb") && requireNamespace("igraph")) {
  # Create synthetic data
  up_mapped <- data.frame(
    Protein = c("TP53", "EGFR"),
    STRING_id = c("9606.ENSP00000269305", "9606.ENSP00000275493")
  )
  down_mapped <- data.frame(
    Protein = c("CALCA", "ACTB"),
    STRING_id = c("9606.ENSP00000302220", "9606.ENSP00000482455")
  )
  interactions_list <- list(up_mapped, down_mapped)

  # Run analysis
  analysis_results <- igraph_analysis(interactions_list, 9606, 400)
  print(analysis_results$Upregulated)
}
```

impute\_data

*Impute Missing Values using Down-Shifted Normal Distribution***Description**

Replaces non-finite (NA, Inf) values in specified LOG2 columns with random values drawn from a normal distribution. This distribution is shifted to a lower mean and narrower standard deviation relative to the observed valid data.

**Usage**

```
impute_data(df, LOG2.names, width = 0.3, downshift = 1.8)
```

**Arguments**

|            |                                                                                                                                                                                 |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df         | A data frame. This frame <b>must</b> contain a logical column named KEEP which specifies the rows to be used for calculating the mean and standard deviation of the valid data. |
| LOG2.names | A character vector of column names (from df) to impute.                                                                                                                         |
| width      | Numeric. The factor by which to shrink the standard deviation of the valid data (e.g., 0.3).                                                                                    |
| downshift  | Numeric. The factor (in standard deviations) by which to shift the mean of the valid data (e.g., 1.8).                                                                          |

**Details**

This method is a common "down-shift" or "Perseus-style" imputation for label-free proteomics, simulating the low-abundance signals of proteins near the detection limit. It assumes missingness is not at random (MNAR).

**Value**

The data frame df with imputed LOG2 columns and new 'impute.\*' logical columns indicating which values were imputed.

**Examples**

```
# Create synthetic LOG2 data with non-finite values (Inf)
log_df <- data.frame(
  Protein = c("ProtA", "ProtB", "ProtC", "ProtD"),
  LOG2.S1 = c(10, 12, Inf, 8),
  LOG2.S2 = c(11, 13, Inf, Inf),
  # Add a KEEP column (e.g., from a filter)
  # Here, we keep all proteins for calculation
  KEEP = c(TRUE, TRUE, TRUE, TRUE)
)

# Specify columns to impute
log_cols <- c("LOG2.S1", "LOG2.S2")

# Run imputation
set.seed(123) # for reproducible example
```

```

imputed_df <- impute_data(log_df, log_cols)

print("Original Data:")
print(log_df)
print("Imputed Data:")
print(imputed_df)

```

---

|                 |                                       |
|-----------------|---------------------------------------|
| impute_KNN_data | <i>Impute missing data using k-NN</i> |
|-----------------|---------------------------------------|

---

## Description

Uses K-Nearest Neighbors (k-NN) to impute missing (NA) values in a log-expression matrix.

## Usage

```
impute_KNN_data(df, LOG2.names, ...)
```

## Arguments

|            |                                                         |
|------------|---------------------------------------------------------|
| df         | A numeric matrix with NA values.                        |
| LOG2.names | A character vector of column names (from df) to impute. |
| ...        | Additional arguments passed to the plot function.       |

## Value

A numeric matrix with NA values imputed.

## Examples

```

log_matrix_na <- matrix(
  c(
    10.0, 10.2, NA, 10.5, 10.1, 9.9, # Sample 1 (with NAs)
    12.0, NA, 11.9, 12.1, 11.8, NA
  ), # Sample 2 (with NAs)
  nrow = 6, ncol = 2,
  dimnames = list(
    c("P1", "P2", "P3", "P4", "P5", "P6"),
    c("Sample1", "Sample2")
  )
)

LOG2.names <- c("Sample1", "Sample2")

imputed_matrix <- impute_KNN_data(as.data.frame(log_matrix_na), LOG2.names)

print(imputed_matrix)

```



---

|                   |                                                             |
|-------------------|-------------------------------------------------------------|
| interactions_down | <i>Plot STRING Interactions for Down-regulated Proteins</i> |
|-------------------|-------------------------------------------------------------|

---

### Description

Maps down-regulated proteins to the STRING database and plots the network.

### Usage

```
interactions_down(df, taxonid, score)
```

### Arguments

|         |                                                                                                     |
|---------|-----------------------------------------------------------------------------------------------------|
| df      | A data frame from statistical analysis (e.g., limma), must have 'expression' and 'Protein' columns. |
| taxonid | Numeric. The NCBI taxonomy ID for the species (e.g., 9606 for human).                               |
| score   | Numeric. The minimum required interaction score (0-1000).                                           |

### Value

This function is called for its side effect of generating a plot. It does not return an object.

### Examples

```
if (requireNamespace("STRINGdb")) {
  # Create synthetic data
  limma_df <- data.frame(
    Protein = c("P10415", "P62258"), # CALCA, ACTB
    expression = c("Down-regulated", "Down-regulated")
  )
  # Run function
  interactions_down(limma_df, taxonid = 9606, score = 400)
}
```

---

|                 |                                                          |
|-----------------|----------------------------------------------------------|
| interactions_up | <i>Get STRING Interactions for Up-regulated Proteins</i> |
|-----------------|----------------------------------------------------------|

---

### Description

Maps up-regulated proteins to the STRING database, plots the network, and returns a list of mapped proteins.

### Usage

```
interactions_up(df, taxonid, score)
```

**Arguments**

|         |                                                                                                     |
|---------|-----------------------------------------------------------------------------------------------------|
| df      | A data frame from statistical analysis (e.g., limma), must have 'expression' and 'Protein' columns. |
| taxonid | Numeric. The NCBI taxonomy ID for the species (e.g., 9606 for human).                               |
| score   | Numeric. The minimum required interaction score (0-1000).                                           |

**Value**

A list containing two data frames: 1. up\_mapped: Mapped up-regulated proteins. 2. down\_mapped: Mapped down-regulated proteins.

**Examples**

```
if (requireNamespace("STRINGdb")) {
  # Create synthetic data
  limma_df <- data.frame(
    Protein = c("P04637", "P00533"), # TP53, EGFR
    expression = c("Up-regulated", "Up-regulated")
  )
  # Run function
  interactions_list <- interactions_up(limma_df, taxonid = 9606, score = 400)
}
```

---

|                  |                                               |
|------------------|-----------------------------------------------|
| median_centering | <i>Perform median centering normalization</i> |
|------------------|-----------------------------------------------|

---

**Description**

Normalizes a numeric matrix of log-expression values by subtracting the median of each column.

**Usage**

```
median_centering(df, LOG2.names)
```

**Arguments**

|            |                                                                   |
|------------|-------------------------------------------------------------------|
| df         | A numeric matrix where rows are proteins and columns are samples. |
| LOG2.names | A vector containing the samples with log2 intensity values.       |

**Value**

A numeric matrix of the same dimensions, now median-centered.

**Examples**

```
# Create a small, synthetic log-expression matrix
log_df <- data.frame(
  Sample1 = c(10.0, 10.2, 9.8),
  Sample2 = c(12.0, 12.1, 11.9)
)
row.names(log_df) <- c("ProtA", "ProtB", "ProtC")

LOG2.names <- c("Sample1", "Sample2")

normalized_df <- median_centering(log_df, LOG2.names)

print(normalized_df)
```

my\_heatmap

*Base R Heatmap***Description**

Creates a heatmap using the base R heatmap function.

**Usage**

```
my_heatmap(data, cond.names, title)
```

**Arguments**

|            |                                                                             |
|------------|-----------------------------------------------------------------------------|
| data       | A data frame containing expression data and a 'Protein' column.             |
| cond.names | A character vector of the column names (samples) to include in the heatmap. |
| title      | A character string for the heatmap's title.                                 |

**Value**

Returns (invisibly) a list with components from the heatmap function, such as rowInd and colInd.

**Examples**

```
# Create synthetic data
heat_data <- data.frame(
  Protein = paste0("Prot", 1:5),
  Sample1 = rnorm(5, 10),
  Sample2 = rnorm(5, 12)
)
sample_names <- c("Sample1", "Sample2")

# Generate the plot
my_heatmap(heat_data, sample_names, "My Heatmap")
```

---

`my_heatmap_differential`*Differential Protein Heatmap (ggplot)*

---

## Description

Creates a ggplot2 heatmap of differentially expressed proteins.

## Usage

```
my_heatmap_differential(limma, data, cond.names, title)
```

## Arguments

|                         |                                                                                                                                |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------|
| <code>limma</code>      | A data frame from statistical analysis, must have 'Protein' and 'expression' columns (e.g., 'Up-regulated', 'Down-regulated'). |
| <code>data</code>       | A data frame containing expression data, must have 'Protein' and sample columns (e.g., LOG2 intensity values).                 |
| <code>cond.names</code> | A character vector of the column names (samples) to include in the heatmap.                                                    |
| <code>title</code>      | A character string for the heatmap's title.                                                                                    |

## Value

A ggplot object.

## Examples

```
# Create synthetic data
limma_results <- data.frame(
  Protein = c("Prot1", "Prot2", "Prot3"),
  expression = c("Up-regulated", "Not Significant", "Down-regulated"),
  logFC = c(2.5, 0.5, -2.1)
)
data_expr <- data.frame(
  Protein = c("Prot1", "Prot2", "Prot3"),
  Sample1 = c(12, 10, 8),
  Sample2 = c(13, 10, 7)
)
sample_names <- c("Sample1", "Sample2")

# Generate the plot
my_heatmap_differential(limma_results, data_expr, sample_names, "DE Heatmap")
```

---

|                    |                                            |
|--------------------|--------------------------------------------|
| normalization_func | <i>Apply Normalization to LOG2 Columns</i> |
|--------------------|--------------------------------------------|

---

## Description

A wrapper function to apply various normalization methods from the `wrMisc` package to the specified LOG2 intensity columns.

## Usage

```
normalization_func(df, LOG2.names, method)
```

## Arguments

|                         |                                                                                                                                                                          |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>df</code>         | A data frame containing the LOG2 expression data.                                                                                                                        |
| <code>LOG2.names</code> | A character vector of column names (from <code>df</code> ) to which the normalization should be applied.                                                                 |
| <code>method</code>     | A character string specifying the normalization method to be passed to <code>wrMisc::normalizeThis</code> . Examples include "median", "mean", "trimMean", "quant", etc. |

## Value

The original data frame (`df`) with the specified `LOG2.names` columns replaced by their normalized versions.

## Examples

```
# Create synthetic LOG2 data
log_df <- data.frame(
  Protein = c("ProtA", "ProtB"),
  LOG2.Sample1 = c(10, 12),
  LOG2.Sample2 = c(11, 13)
)

# Specify which columns to normalize
log_cols <- c("LOG2.Sample1", "LOG2.Sample2")

# Run median normalization
normalized_df <- normalization_func(log_df, log_cols, "median")

print("Original Data:")
print(log_df)
print("Normalized Data:")
print(normalized_df)
```

---

|                  |                                 |
|------------------|---------------------------------|
| obtain_LOG.names | <i>Obtain LOG2 Column Names</i> |
|------------------|---------------------------------|

---

**Description**

A helper function to find all column names containing "LOG2".

**Usage**

```
obtain_LOG.names(df)
```

**Arguments**

df                      A data.frame to search.

**Value**

A character vector of column names.

**Examples**

```
# Create a small example data frame
my_df <- data.frame(
  Protein = c("P1", "P2"),
  Intensity.A = c(100, 200),
  LOG2.A = c(6.6, 7.6),
  Intensity.B = c(110, 210),
  LOG2.B = c(6.7, 7.7)
)

# This example is runnable!
log_names <- obtain_LOG.names(my_df)
print(log_names)
```

---

|                        |                                                  |
|------------------------|--------------------------------------------------|
| obtain_unique_proteins | <i>Obtain Unique Proteins Between Conditions</i> |
|------------------------|--------------------------------------------------|

---

**Description**

Identifies proteins that are uniquely present in one of two conditions, based on the presence of finite (e.g., LOG2 intensity) vs. non-finite (e.g., Inf, NA) values.

**Usage**

```
obtain_unique_proteins(df, metadata, selected_conditions)
```

**Arguments**

|                     |                                                                                              |
|---------------------|----------------------------------------------------------------------------------------------|
| df                  | A data frame containing expression data, with LOG2 intensity columns and a 'Protein' column. |
| metadata            | A data frame with sample metadata. Must have 'group' and 'log2_col' columns.                 |
| selected_conditions | A character vector of length 2 specifying the two groups from the 'group' column to compare. |

**Details**

This function is designed for label-free data where a protein's absence is marked by a non-finite value (like Inf from a log-transformation of 0). It identifies proteins present in at least half of the replicates of one condition while being completely absent (non-finite) in the other.

**Value**

A list containing two data frames: 1. cond1\_unicas: A data frame of proteins unique to the first group. 2. cond2\_unicas: A data frame of proteins unique to the second group.

**Examples**

```
# Create synthetic data with infinite values (representing missing)
df_prot <- data.frame(
  Protein = paste0("Prot", 1:4),
  LOG2.C1 = c(10, 12, Inf, 9),
  LOG2.C2 = c(11, 13, Inf, 10),
  LOG2.T1 = c(Inf, Inf, 8, 11),
  LOG2.T2 = c(Inf, Inf, 7, 12)
)
# Prot1/2 are present in Control, absent in Treatment
# Prot3 is present in Treatment, absent in Control
# Prot4 is present in both

metadata <- data.frame(
  log2_col = c("LOG2.C1", "LOG2.C2", "LOG2.T1", "LOG2.T2"),
  group = c("Control", "Control", "Treatment", "Treatment")
)
# Note: T is [1] (second_group), C is [2] (first_group)
selected_cond <- c("Treatment", "Control")

unique_list <- obtain_unique_proteins(df_prot, metadata, selected_cond)

# cond1_unicas (Control) should have Prot1, Prot2
print("Unique to Control:")
print(unique_list[[1]]$Protein)

# cond2_unicas (Treatment) should have Prot3
print("Unique to Treatment:")
print(unique_list[[2]]$Protein)
```

---

pca *Custom PCA Plot (Base R)*

---

**Description**

Performs PCA and generates a 2D scatter plot of the first two principal components using base R plotting.

**Usage**

```
pca(x, metadata, selected_conditions, pc_x = 1, pc_y = 2)
```

**Arguments**

|                     |                                                                                                                                    |
|---------------------|------------------------------------------------------------------------------------------------------------------------------------|
| x                   | A data frame or matrix with expression data. Columns are samples (e.g., LOG2 intensity values). Rows are features (e.g. proteins). |
| metadata            | A data frame with sample metadata. Must have 'group' and 'log2_col' columns.                                                       |
| selected_conditions | A character vector of length 2 specifying the two groups from the 'group' column to compare.                                       |
| pc_x                | Principal component for X axis.                                                                                                    |
| pc_y                | Principal component for Y axis.                                                                                                    |

**Value**

This function is called for its side effect of generating a base R plot. It does not return an object.

**Examples**

```
# Create synthetic data
x_data <- data.frame(
  LOG2.C1 = rnorm(10, 8), LOG2.C2 = rnorm(10, 8),
  LOG2.T1 = rnorm(10, 9), LOG2.T2 = rnorm(10, 9),
  row.names = paste0("Prot", 1:10)
)
metadata <- data.frame(
  log2_col = c("LOG2.C1", "LOG2.C2", "LOG2.T1", "LOG2.T2"),
  group = c("Control", "Control", "Treatment", "Treatment")
)
selected_cond <- c("Treatment", "Control") # Matches user's logic [2] then [1]

# Generate the plot
pca(x_data, metadata, selected_cond)
```



plotCV2

*Plot Coefficient of Variation vs. Mean***Description**

Generates a plot of the squared Coefficient of Variation (CV) versus the mean abundance (A). This is often used to check imputation quality.

**Usage**

```
plotCV2(y, trend = TRUE, main = "Imputation check", ...)
```

**Arguments**

|       |                                                                                                               |
|-------|---------------------------------------------------------------------------------------------------------------|
| y     | A numeric data frame or matrix where rows are features (proteins) and columns are samples (LOG2 intensities). |
| trend | Logical. If TRUE, a <code>limma::loessFit</code> trendline is added to the plot.                              |
| main  | Character. The main title for the plot.                                                                       |
| ...   | Additional arguments passed to the plot function.                                                             |

**Value**

A data frame containing the mean (A) and CV ( $CV^2$ ) values that were plotted.

**Examples**

```
# Create synthetic LOG2 intensity data
log_data <- matrix(rnorm(100, mean = 10, sd = 1), nrow = 20, ncol = 5)
log_data[sample(1:100, 10)] <- NA # Add some NAs

# Create the CV plot
cv_data <- plotCV2(log_data, main = "CV vs. Mean Plot")
print(head(cv_data))
```

postimputation\_state

*Plot Post-Imputation Density***Description**

Plots the density of intensity values before and after imputation to visualize the effect of the imputation.

**Usage**

```
postimputation_state(data_filtered, imputation, LOG2.names)
```

**Arguments**

`data_filtered` The data frame *before* imputation, containing non-finite values (NA, Inf).  
`imputation` An indicator (1 or 2) specifying the imputation method. 1 = `impute_KNN_data`, 2 = `impute_data`.  
`LOG2.names` A character vector of the LOG2 column names to use.

**Value**

A ggplot object showing the two density plots.

**Examples**

```
# This function depends on `impute_KNN_data` and `impute_data`
# We must create those functions and the data they need.

# 1. Create synthetic data
data_filt <- data.frame(
  Protein = c("A", "B", "C", "D"),
  LOG2.S1 = c(10, 12, NA, 8),
  LOG2.S2 = c(11, 13, 9, NA),
  KEEP = c(TRUE, TRUE, TRUE, TRUE) # For impute_data
)

# 2. Create minimal versions of the imputation functions for the example
impute_KNN_data <- function(df, lnames, k) {
  df[lnames][is.na(df[lnames])] <- mean(unlist(df[lnames]), na.rm = TRUE)
  return(df)
}
impute_data <- function(df, lnames) {
  df[lnames][is.na(df[lnames])] <- rnorm(sum(is.na(df[lnames])), mean = 7, sd = 0.3)
  return(df)
}

# 3. Run the plot function
postimputation_state(data_filt, imputation = 2, LOG2.names = c("LOG2.S1", "LOG2.S2"))
```

---

`preimputation_state`     *Plot Missingness Pattern*

---

**Description**

Generates a missing value aggregation plot from the VIM package to visualize patterns of missing data.

**Usage**

```
preimputation_state(df, cond.names)
```

**Arguments**

`df` A data frame containing the data to be plotted.  
`cond.names` A character vector of column names from `df` to be included in the missingness plot.

**Value**

A plot showing the aggregation of missing values.

**Examples**

```
# Create synthetic data with NAs
log_df <- data.frame(
  LOG2.C1 = c(10, 10.1, NA, 9.9),
  LOG2.C2 = c(11, NA, NA, 11.2),
  LOG2.T1 = c(12, 12.1, 12.2, 12.3)
)

# Plot the missingness pattern
preimputation_state(log_df, c("LOG2.C1", "LOG2.C2", "LOG2.T1"))
```

---

|                 |                   |
|-----------------|-------------------|
| qqplot_function | Create a Q-Q Plot |
|-----------------|-------------------|

---

**Description**

Generates a Q-Q plot to compare the distributions of two columns in a data frame.

**Usage**

```
qqplot_function(df, colname1, colname2, color)
```

**Arguments**

|          |                                                   |
|----------|---------------------------------------------------|
| df       | A data frame.                                     |
| colname1 | Character. The name of the column for the x-axis. |
| colname2 | Character. The name of the column for the y-axis. |
| color    | The color for the points.                         |

**Value**

A ggplot object.

**Examples**

```
my_data <- data.frame(
  Theoretical = rnorm(100),
  Sample = rnorm(100, mean = 0.5)
)
qqplot_function(my_data, "Theoretical", "Sample", "blue")
```

---

|                 |                             |
|-----------------|-----------------------------|
| quick_filtering | <i>Quick Data Filtering</i> |
|-----------------|-----------------------------|

---

**Description**

Filters raw proteomics data (e.g., from MaxQuant) to remove contaminants, reverse hits, and site-only identifications. It also parses protein identifiers from Fasta headers.

**Usage**

```
quick_filtering(
  raw,
  platform,
  organism,
  metadata,
  selected_conditions,
  directory_path = NULL
)
```

**Arguments**

|                     |                                                                   |
|---------------------|-------------------------------------------------------------------|
| raw                 | A data frame of raw proteomics data (e.g., from MaxQuant).        |
| platform            | An indicator (e.g., 1) for the data platform (e.g., MaxQuant).    |
| organism            | An indicator (e.g., 1 for Human, 2 for Mouse, etc.).              |
| metadata            | A data frame mapping intensity column names to sample names.      |
| selected_conditions | (Not currently used in function) A vector of selected conditions. |
| directory_path      | (Not currently used in function) A path to a directory.           |

**Value**

A data frame filtered to remove contaminants/reverse hits, with new "Protein" and "Protein\_description" columns.

**Examples**

```
raw_data <- data.frame(
  Potential.contaminant = c("", "+", "", ""),
  Reverse = c("", "", "+", ""),
  Only.identified.by.site = c("", "", "", "+"),
  Fasta.headers = c(
    ">sp|P04637|P53_HUMAN Cellular tumor antigen p53 OS=Homo sapiens",
    ">sp|P00000|CONTAM_Protein Common contaminant",
    ">sp|P12345|REV_Protein Reverse Sequence",
    ">sp|P62258|1433E_HUMAN 14-3-3 protein epsilon"
  ),
  # Intensity columns
  Intensity.S1 = c(10000, 500, 200, 100),
  Intensity.S2 = c(12000, 600, 150, 90),
  stringsAsFactors = FALSE
)
```

```

metadata <- data.frame(
  intensity_sample_name = c("Intensity.S1", "Intensity.S2"),
  sample_name = c("Sample_A", "Sample_B")
)

filtered_df <- quick_filtering(
  raw = raw_data,
  platform = 1,
  organism = 2,
  metadata = metadata,
  selected_conditions = NULL,
  directory_path = NULL
)

```

runTraianProt

*Launch the TraianProt Shiny Application***Description**

This function builds and returns the Shiny app object for TraianProt.

**Usage**

```
runTraianProt()
```

**Value**

A shiny.appobj object representing the TraianProt app.

**Examples**

```

app <- runTraianProt()

if (interactive()) {
  shiny::runApp(app)
}

```

scatterplot\_function

*Create a Scatterplot with Marginal Densities***Description**

Uses ggplot2 and ggExtra to create a scatterplot comparing two columns, with marginal density plots.

**Usage**

```
scatterplot_function(df, colname1, colname2)
```

**Arguments**

|          |                                                   |
|----------|---------------------------------------------------|
| df       | A data frame.                                     |
| colname1 | Character. The name of the column for the x-axis. |
| colname2 | Character. The name of the column for the y-axis. |

**Value**

A ggExtra plot object.

**Examples**

```
my_data <- data.frame(  
  Sample1 = rnorm(100),  
  Sample2 = rnorm(100)  
)  
scatterplot_function(my_data, "Sample1", "Sample2")
```

---

statistical\_analysis    *Limma function for statistical analysis*

---

**Description**

A comprehensive function to perform differential expression (DE) analysis between two conditions. It supports t-tests, Wilcoxon tests, and limma, with options for paired data and DEqMS spectral count weighting.

**Usage**

```
statistical_analysis(  
  df,  
  test,  
  paired = FALSE,  
  metadata,  
  logfc,  
  sig,  
  adjval,  
  statval,  
  unique_proteins,  
  way,  
  psms,  
  platform,  
  selected_conditions,  
  diann_dir = NULL  
)
```

**Arguments**

|                                  |                                                                                                                                                                        |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>df</code>                  | The primary data frame containing expression data (rows=proteins, cols=samples). Must also contain 'Protein' and 'Protein_description' columns.                        |
| <code>test</code>                | Numeric. The statistical test to use: 1 for <code>t.test</code> , 2 for <code>limma</code> , 3 for <code>wilcox.test</code> .                                          |
| <code>paired</code>              | Logical. TRUE if the experimental design is paired, FALSE otherwise.                                                                                                   |
| <code>metadata</code>            | A data frame with sample metadata. Must contain group (condition) and <code>log2_col</code> (sample names matching <code>df</code> colnames).                          |
| <code>logfc</code>               | Numeric. The log-fold change (LFC) threshold for 'Up-regulated' and 'Down-regulated' status.                                                                           |
| <code>sig</code>                 | Numeric. The significance threshold (e.g., 0.05) to be used with <code>statval</code> .                                                                                |
| <code>adjval</code>              | String. The p-value adjustment method for <code>p.adjust</code> (e.g., "BH").                                                                                          |
| <code>statval</code>             | Numeric. Which p-value to use for significance: 1 for raw p-value, 2 for adjusted p-value.                                                                             |
| <code>unique_proteins</code>     | A list with two elements containing proteins unique to the control ( <code>[1]</code> ) and treatment ( <code>[2]</code> ) groups. Used only if <code>way = 2</code> . |
| <code>way</code>                 | Numeric. 1 to analyze only shared proteins, 2 to include unique proteins from <code>unique_proteins</code> .                                                           |
| <code>psms</code>                | Logical. If <code>test = 2</code> (limma), TRUE to use DEqMS for spectral count weighting.                                                                             |
| <code>platform</code>            | Numeric. Used if <code>psms = TRUE</code> . Specifies data source for finding PSM columns: 1=MaxQuant, 2=MSFragger, 4=Proteome Discoverer.                             |
| <code>selected_conditions</code> | A character vector of length 2. <code>selected_conditions[2]</code> is treated as the control group, and <code>selected_conditions[1]</code> as the treatment group.   |
| <code>diann_dir</code>           | String. Directory path for DIA-NN. <b>Note:</b> This parameter is currently not implemented in the function body.                                                      |

**Details**

Perform Differential Expression Statistical Analysis

This function acts as a wrapper for various statistical tests. The logFC is calculated as `mean(treatment) - mean(control)`.

When `way = 2`, unique proteins are added to the results with imputed logFC and p-values (e.g., `p-value = min(p.value)/100`) to ensure they appear in visualizations.

The function uses several non-standard variable assignment methods (e.g., `assign`, `ls`, `get`) to dynamically create sample groups.

**Value**

A data frame (`results.eb`) with DE results, including logFC, p.value, adj.P.Val, expression, Protein, and Protein\_description. Additional columns may be present for limma/DEqMS (e.g., `sca.P.Value`).

**Examples**

```
# 1. Create a mock data frame (df)
set.seed(123)
df_data <- data.frame(
  Protein = paste0("Prot", 1:5),
  Protein_description = paste("Description for", paste0("Prot", 1:5)),
  Cond1_R1 = rnorm(5, 10, 1),
  Cond1_R2 = rnorm(5, 10, 1),
  Cond2_R1 = rnorm(5, 12, 1), # Cond2 is higher
  Cond2_R2 = rnorm(5, 12, 1)
)
rownames(df_data) <- df_data$Protein

# 2. Create mock metadata
meta <- data.frame(
  log2_col = c("Cond1_R1", "Cond1_R2", "Cond2_R1", "Cond2_R2"),
  group = c("Condition1", "Condition1", "Condition2", "Condition2")
)

# 3. Define unique proteins (for way = 2)
uniques_list <- list(
  data.frame(Protein = "Prot_Control", Protein_description = "Only in Control"),
  data.frame(Protein = "Prot_Treat", Protein_description = "Only in Treatment")
)

# Run analysis (t-test, unpaired, no PSMs, include uniques)
results <- statistical_analysis(
  df = df_data,
  test = 1, # t-test
  paired = FALSE,
  metadata = meta,
  logfc = 1,
  sig = 0.05,
  adjval = "BH",
  statval = 2, # Use adjusted p-value
  unique_proteins = uniques_list,
  way = 2, # Include uniques
  psms = FALSE,
  platform = 1,
  selected_conditions = c("Condition2", "Condition1") # Treat 2 vs 1
)

print(results)
```

---

traianprot\_power\_curve

*Create power curve*


---

**Description**

Calculates the theoretical power curve based on the observed variability in the experimental data and a desired Fold Change.



**Usage**

```
traianprot_power_curve(
  df,
  log2_cols,
  foldchange,
  replicatespower,
  alpha_level_choice,
  alpha_level
)
```

**Arguments**

|                    |                                                                                                                    |
|--------------------|--------------------------------------------------------------------------------------------------------------------|
| df                 | A data.frame or matrix containing the expression data.                                                             |
| log2_cols          | Character vector or numeric indices indicating which columns of df contain the abundance values (must be numeric). |
| foldchange         | Numeric. The expected Fold Change to calculate the power (e.g., 2 for doubling, 0.5 for halving).                  |
| replicatespower    | Numeric. Number of replicates per group.                                                                           |
| alpha_level_choice | Numeric. Choice to consider either p-value or adjusted p-value.                                                    |
| alpha_level        | Numeric. Global significance level before correction (defaults to 0.05).                                           |

**Value**

A ggplot object containing the power curve.

**Examples**

```
# Simulated data
data <- data.frame(
  ID = letters[1:10],
  R1 = rnorm(10), R2 = rnorm(10), R3 = rnorm(10)
)
plot <- traianprot_power_curve(
  data, c("R1", "R2", "R3"),
  foldchange = 2,
  replicatespower = 5,
  alpha_level_choice = 1,
  alpha_level = 0.05
)
print(plot)
```

---

traian\_to\_SE

---

*Export TraianProt results to SummarizedExperiment*


---

**Description**

Compiles the raw, normalized, and statistical results from the TraianProt pipeline into a Bioconductor-standard SummarizedExperiment object.

**Usage**

```
traian_to_SE(df.F, total_dataset, metadata, df_limma)
```

**Arguments**

|               |                                                         |
|---------------|---------------------------------------------------------|
| df.F          | dataframe from preprocessing methods.                   |
| total_dataset | whole dataframe including absence and presence proteins |
| metadata      | metadata that defines the experiment                    |
| df_limma      | dataframe containing statistical results                |

**Value**

a Bioconductor-standard SummarizedExperiment object, containing the raw, normalized and statistical results.

**Examples**

```
df_raw <- data.frame(
  Protein = paste0("Protein_", 1:5),
  WT_1 = runif(5, 100, 1000), WT_2 = runif(5, 100, 1000),
  Treat_1 = runif(5, 100, 1000), Treat_2 = runif(5, 100, 1000)
)

df_norm <- df_raw
df_norm[, 2:5] <- log2(df_norm[, 2:5]) # Simulamos la normalización

meta <- data.frame(
  Condition = c("WT", "WT", "Treatment", "Treatment"),
  log2_col = c("WT_1", "WT_2", "Treat_1", "Treat_2")
)

stats <- data.frame(
  Protein = paste0("Protein_", 1:5),
  logFC = c(1.2, -0.5, 2.1, 0.1, -1.8),
  p_value = c(0.01, 0.4, 0.005, 0.8, 0.02)
)

se_object <- traian_to_SE(df_raw, df_norm, meta, stats)
se_object
```

tsne

*t-SNE Plot***Description**

Generates a t-SNE plot for sample clustering using ggplot2.

**Usage**

```
tsne(x, metadata, perplexity_num, selected_conditions)
```

**Arguments**

|                     |                                                                                                                                    |
|---------------------|------------------------------------------------------------------------------------------------------------------------------------|
| x                   | A data frame or matrix with expression data. Columns are samples (e.g., LOG2 intensity values). Rows are features (e.g. proteins). |
| metadata            | A data frame with sample metadata. Must have 'group' and 'log2_col' columns.                                                       |
| perplexity_num      | Numeric. The perplexity value for the t-SNE algorithm.                                                                             |
| selected_conditions | A character vector of length 2 specifying the two groups from the 'group' column to compare.                                       |

**Value**

A ggplot object.

**Examples**

```
df <- data.frame(
  # Group A (Low values)
  Sample1 = c(10.1, 10.5, 12.0, 10.0),
  Sample2 = c(10.2, 10.6, 12.1, 10.1),
  Sample3 = c(10.3, 10.7, 12.2, 10.2),
  Sample4 = c(10.4, 10.8, 12.3, 10.3),
  Sample5 = c(10.5, 10.9, 12.4, 10.4),
  # Group B (High values)
  Sample6 = c(20.1, 21.5, 22.0, 20.0),
  Sample7 = c(20.2, 21.6, 22.1, 20.1),
  Sample8 = c(20.3, 21.7, 22.2, 20.2),
  Sample9 = c(20.4, 21.8, 22.3, 20.3),
  Sample10 = c(20.5, 21.9, 22.4, 20.4)
)
row.names(df) <- c("P1", "P2", "P3", "P4")

metadata <- data.frame(
  log2_col = paste0("Sample", 1:10),
  group = c(rep("A", 5), rep("B", 5))
)
selected_conditions <- c("A", "B")

if (requireNamespace("Rtsne") && requireNamespace("ggplot2")) {
  tsne_plot <- tsne(
    x = df,
    metadata = metadata,
    perplexity_num = 2,
    selected_conditions = selected_conditions
  )

  print(tsne_plot)
}
```

## Description

Filters a protein data frame based on a minimum number of unique peptides found in a minimum fraction of replicates per condition.

## Usage

```
unique_peptides_filter(df, metadata, number, min_fraction)
```

## Arguments

|              |                                                                                                                                                                        |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| df           | A data frame with protein data. Must have rownames (e.g., Protein IDs) and columns corresponding to unique peptide counts.                                             |
| metadata     | A metadata data frame. Must contain 'group' and 'unique_peptides_col' columns to map samples to groups.                                                                |
| number       | Numeric. The minimum number of unique peptides (e.g., 1 or 2) required to count as 'present' in a single sample.                                                       |
| min_fraction | Numeric. The minimum fraction (0 to 1) of replicates in <i>at least one</i> group that must meet the 'number' threshold. (e.g., 0.5 means at least 50% of replicates). |

## Details

This function is useful for filtering data (e.g., from MaxQuant) to remove proteins with low confidence. It keeps a protein if, for **at least one** experimental group (condition), the unique peptide count is  $\geq$  number in at least min\_fraction of the samples in that group.

## Value

A data frame (df\_filtered) containing only the rows (proteins) that pass the filter.

## Examples

```
# Create synthetic data
peptide_df <- data.frame(
  Pep.C1 = c(2, 0, 1, 5),
  Pep.C2 = c(3, 1, 0, 6),
  Pep.T1 = c(0, 2, 1, 0),
  Pep.T2 = c(0, 3, 0, 0)
)
rownames(peptide_df) <- c("ProtA", "ProtB", "ProtC", "ProtD")

meta <- data.frame(
  unique_peptides_col = c("Pep.C1", "Pep.C2", "Pep.T1", "Pep.T2"),
  group = c("Control", "Control", "Treatment", "Treatment")
)

# Filter: require min 1 peptide in at least 75% of reps (i.e., 2/2)
# ProtA: Passes in Control (2/2 have  $\geq$  1). Kept.
# ProtB: Passes in Treatment (2/2 have  $\geq$  1). Kept.
# ProtC: Fails in Control (1/2), Fails in Treatment (1/2). Dropped.
# ProtD: Passes in Control (2/2 have  $\geq$  1). Kept.

filtered_df <- unique_peptides_filter(
  df = peptide_df,
  metadata = meta,
```

```

        number = 1,
        min_fraction = 0.75
    )

    print("Filtered proteins (should be A, B, D):")
    print(rownames(filtered_df))

```

venn\_diagram

*Create a Venn Diagram***Description**

Generates a Venn diagram plot object from a list of unique proteins and a data frame of common proteins.

**Usage**

```
venn_diagram(df, unique_proteins, color1, color2)
```

**Arguments**

|                 |                                                                                                               |
|-----------------|---------------------------------------------------------------------------------------------------------------|
| df              | A data frame of common proteins (must have a "Protein" column).                                               |
| unique_proteins | A list containing two data frames: 1. Proteins unique to the first set. 2. Proteins unique to the second set. |
| color1          | Color for the first set.                                                                                      |
| color2          | Color for the second set.                                                                                     |

**Value**

A gList object (a plot) representing the Venn diagram.

**Examples**

```

common_proteins <- data.frame(
  Protein = c("ProteinA", "ProteinB", "ProteinC")
)

unique_protein_list <- list(
  Control = data.frame(Protein = c("ProteinD", "ProteinE")),
  Treatment = data.frame(Protein = c("ProteinF", "ProteinG", "ProteinH", "ProteinI"))
)

my_venn_plot <- venn_diagram(
  df = common_proteins,
  unique_proteins = unique_protein_list,
  color1 = "blue",
  color2 = "red"
)

grid::grid.newpage()
grid::grid.draw(my_venn_plot)

```

---

|              |                                                                                                                                 |
|--------------|---------------------------------------------------------------------------------------------------------------------------------|
| volcano_plot | <i>This function generates an interactive volcano plot using the 'plotly' package based on differential expression results.</i> |
|--------------|---------------------------------------------------------------------------------------------------------------------------------|

---

## Description

This function generates an interactive volcano plot using the 'plotly' package based on differential expression results.

## Usage

```
volcano_plot(limma, title, label, statval, psms)
```

## Arguments

|         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| limma   | <p>A data frame containing differential expression results. This data frame must include columns:</p> <ul style="list-style-type: none"> <li>• logFC: Log-fold change values.</li> <li>• Protein: Protein identifiers (used for hover-text).</li> <li>• expression: A character vector (e.g., "Up-regulated", "Down-regulated", "Unchanged") used for coloring.</li> <li>• p.value or sca.P.Value: Nominal p-values.</li> <li>• adj.P.Val or sca.adj.pval: Adjusted p-values.</li> </ul> |
| title   | A character string for the plot title.                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| label   | A numeric value specifying the size of the markers (points) in the plot. Passed to size = I(label).                                                                                                                                                                                                                                                                                                                                                                                      |
| statval | <p>A numeric value (1 or 2) specifying which p-value to plot on the y-axis.</p> <ul style="list-style-type: none"> <li>• 1: Plots the nominal p-value (e.g., p.value or sca.P.Value).</li> <li>• 2: Plots the adjusted p-value (e.g., adj.P.Val or sca.adj.pval).</li> </ul>                                                                                                                                                                                                             |
| psms    | <p>A logical value (TRUE or FALSE).</p> <ul style="list-style-type: none"> <li>• TRUE: Uses PSM-aware p-values from DEqMS (i.e., sca.P.Value or sca.adj.pval).</li> <li>• FALSE: Uses standard p-values (i.e., p.value or adj.P.Val).</li> </ul>                                                                                                                                                                                                                                         |

## Details

The function selects the appropriate p-value column based on the statval and psms arguments. The y-axis label is automatically set to "-log10 p-value" or "-log10 q-value" (for adjusted p-values). Points are colored based on the expression column.

## Value

A plotly object, which renders as an interactive volcano plot.

## Examples

```
# Create a mock data frame for demonstration
limma_results <- data.frame(
  logFC = rnorm(100, 0, 2),
  Protein = paste0("PROT", 1:100),
  p.value = runif(100, 0, 1),
  adj.P.Val = runif(100, 0, 1),
  sca.P.Value = runif(100, 0, 1),
  sca.adj.pval = runif(100, 0, 1),
  expression = sample(c("Up-regulated", "Down-regulated", "Unchanged"),
    100,
    replace = TRUE
  )
)

# Generate an interactive plot using adjusted p-values without PSM weighting
volcano_plot(
  limma = limma_results,
  title = "Interactive Volcano Plot",
  label = 5,
  statval = 2,
  psms = FALSE
)
```

---

volcano\_plot\_tiff

Create a Static Volcano Plot for Publication

---

## Description

This function generates a static volcano plot using the 'ggplot2' package, suitable for saving as a high-resolution image (e.g., TIFF) for publication.

## Usage

```
volcano_plot_tiff(limma, title, label, statval, psms)
```

## Arguments

- |       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|-------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| limma | A data frame containing differential expression results. This data frame must include columns: <ul style="list-style-type: none"> <li>• logFC or log2FC: Log-fold change values.</li> <li>• Protein: Protein identifiers.</li> <li>• expression: A character vector (e.g., "Up-regulated", "Down-regulated", "Unchanged") used for coloring.</li> <li>• p.value or sca.P.Value: Nominal p-values.</li> <li>• adj.P.Val or sca.adj.pval: Adjusted p-values.</li> </ul> |
| title | A character string for the plot title.                                                                                                                                                                                                                                                                                                                                                                                                                                |
| label | A numeric value specifying the size of the points. <b>Note:</b> In the current function, this parameter is only used when statval = 1 and psms = TRUE. In all other cases, the size is hard-coded to 2.                                                                                                                                                                                                                                                               |

- statval** A numeric value (1 or 2) specifying which p-value to plot on the y-axis.
- 1: Plots the nominal p-value (e.g., `p.value` or `sca.P.Value`).
  - 2: Plots the adjusted p-value (e.g., `adj.P.Val` or `sca.adj.pval`).
- psms** A logical value (TRUE or FALSE).
- TRUE: Uses PSM-aware p-values from DEqMS (i.e., `sca.P.Value` or `sca.adj.pval`).
  - FALSE: Uses standard p-values (i.e., `p.value` or `adj.P.Val`).

## Details

The function uses `ggplot2::theme_light()` and customizes axis text and line sizes. The y-axis label is automatically set to "-log10 p-value" or "-log10 q-value" (for adjusted p-values).

## Value

A ggplot object, which renders as a static volcano plot.

## Examples

```
mock_fc <- rnorm(100, 0, 2)

limma_results <- data.frame(
  logFC = mock_fc,
  log2FC = mock_fc, # Use the vector we just created
  Protein = paste0("PROT", 1:100),
  p.value = runif(100, 0, 1),
  adj.P.Val = runif(100, 0, 1),
  sca.P.Value = runif(100, 0, 1),
  sca.adj.pval = runif(100, 0, 1),
  expression = sample(c("Up-regulated", "Down-regulated", "Unchanged"),
    100,
    replace = TRUE
  )
)

# Generate a static plot
static_plot <- volcano_plot_tiff(
  limma = limma_results,
  title = "Static Volcano Plot",
  label = 3,
  statval = 2,
  psms = TRUE
)

print(static_plot)
```



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