Package 'amanida'

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Title Meta-Analysis for Non-Integral Data

Version 0.3.0

Description Combination of results for meta-analysis using significance and effect size only. P-values and fold-change are combined to obtain a global significance on each metabolite. Produces a volcano plot summarising the relevant results from meta-analysis. Vote-counting reports for metabolites. And explore plot to detect discrepancies between studies at a first glance. Methodology is described in the Llambrich et al. (2021) <doi:10.1093/bioinformatics/btab591>.

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URL `https://github.com/mariallr/amanida`

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Author Maria Llambrich [aut, cre] (<`https://orcid.org/0000-0001-8418-0982`>),
Eudald Correig [aut],
Raquel Cumeras [aut]

Maintainer Maria Llambrich <`maria.llambrich@urv.cat`>

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R topics documented:

`amanida` *amanida*

Description

amanida: A package for Meta-Analysis with non-integral data

Author(s)

Maria Llambrich, Eudald Correig and Raquel Cumeras

Results combination for meta-analysis using only significance and effect size.

- P-values and fold-change are combined to obtain a global significance on each metabolite.
- Produces a volcano plot summarizing the relevant results from meta-analysis.
- Qualitative meta-analysis for metabolites
- Graphical representation of qualitative analysis by bar plot
- Trend explore plot to detect discrepancies between studies at a first glance

See Also

Useful links:

- `https://github.com/mariallr/amanida`

`amanida_palette` *Get nice colour-blind colours*

Description

Get nice colour-blind colours

Usage

```
amanida_palette()
```

Value

vector of colours

`amanida_read` *Import data*

Description

`amanida_read` imports the data and formats for `compute_amanida` or `amanida_vote` functions

Usage

```
amanida_read(file, mode, coln, separator = NULL)
```

Arguments

`file`	path to file
`mode`	indicate if data will be quantitative or qualitative. Options are: • "quan" for quantitative meta-analysis using p-value and fold-change • "qual" for qualitative meta-analysis using trend label
`coln`	columns names to use. It has to be in order identification, p-values, fold-changes, sample size and reference.
`separator`	the separator used on file

Details

Note that `amanida_read` skips rows with missing values or NA. Negatives values for fold-change are transformed to positive (1/value).

Formats compatible are csv, xlsx, xls or txt.

Value

tibble table with data imported

Examples

```
coln <-  c("Compound Name", "P-value", "Fold-change", "N total", "References")
input_file <- getsampleDB()
datafile <- amanida_read(input_file, mode = "quan", coln, separator=";")
```

`amanida_report` *Report*

Description

`amanida_report` creates a report from the data using amanida functions

Usage

```
amanida_report(
  input_file,
  separator = NULL,
  analysis_type = NULL,
  column_id,
  pvalue_cutoff = NULL,
  fc_cutoff = NULL,
  votecount_lim,
  path = NULL,
  comp_inf = NULL
)
```

Arguments

`input_file`	path to the original dataset in xlsx, xls, csv or txt format
`separator`	indicate the separator used in the input_file parameter
`analysis_type`	indicate if data will be quantitative, qualitative or both. Options are: • "quan-qual" for quantitative and qualitative meta-analysis • "quan" for quantitative meta-analysis using p-value and fold-change • "qual" for qualitative meta-analysis using trend label
`column_id`	vector containing columns names to use. It has to be in order identification, p-values, fold-changes, sample size and reference.
`pvalue_cutoff`	numeric value to consider statistical significance
`fc_cutoff`	numeric value to consider significance for effect size
`votecount_lim`	minimum numeric value for vote-counting visualization
`path`	path to the directory where html file is created, otherwise the file will be saved in a temporal folder
`comp_inf`	name checking using information from public databases

Details

This function uses directly the dataset to create a report with the meta-analysis results. In case of quantitative analysis `amanida_report` uses the functions `amanida_read` and `compute_amanida` for analyse the input data. Then the results are showed using `volcano_plot`, `explore_plot` and `vote_plot`.

Value

an html document saved in the working directory

Examples

```
## Not run:
column_id = c("Compound Name", "P-value", "Fold-change", "N total", "References")
input_file <- getsampleDB()

amanida_report(input_file, separator = ";", column_id, analysis_type = "quan",
                pvalue_cutoff = 0.05, fc_cutoff = 4, votecount_lim = 2,
                comp_inf = F)

## End(Not run)
```

`amanida_vote` *Qualitative meta-analysis*

Description

`amanida_vote` performs vote-counting on qualitative data.

Usage

```
amanida_vote(data)
```

Arguments

`data`	data imported using `amanida_read` function w/o names checked by `check_names`

Details

Vote-counting is computed without trend division. Punctuation of entries is based on trend, up-regulation gives 1, down-regulation give -1 and equal behavior gives 0. Total sum is divided then by the total number of entries on each compound. Compound combination is made with PubChem CID when is available.

Note that `amanida_vote` skips rows with missing values or NA.

Formats compatible are csv, xlsx, xls or txt.

Value

METAtable S4 object with vote-counting for each compound on @slot vote

Examples

```
## Not run:
coln = c("Compound Name", "Behaviour", "References")
input_file <- system.file("extdata", "dataset2.csv", package = "amanida")
data_votes <- amanida_read(input_file, mode = "qual", coln, separator = ";")

vote_result <- amanida_vote(data_votes)

## End(Not run)
```

`check_names` *Amanida harmonization*

Description

`check_names` check the names to harmonize them to a common nomenclature. Valid names are: chemical name, InChI, InChIKey and SMILES.

Usage

```
check_names(data)
```

Arguments

`data`	data imported using `amanida_read` function

Details

Note that `check_names` depends on `webchem`package and it slows down the process.

Formats compatible are `amanida_read` output

Value

tibble table with data imported with PubChem ID retrieved

Examples

```
## Not run:
coln <-  c("Compound Name", "P-value", "Fold-change", "N total", "References")
input_file <- getsampleDB()
datafile <- amanida_read(input_file, mode = "quan", coln, separator=";")

data_checked <- check_names(datafile)
```

```
## End(Not run)
```

`compute_amanida` *Combine statistical results and compute vote-counting*

Description

`compute_amanida` Combines for the same entry or metabolite the statistical values of p-value and fold-change. Also is computed a vote-counting for each compound. Compound combination is made with PubChem CID when is available.

Usage

```
compute_amanida(datafile, comp.inf = F)
```

Arguments

`datafile`	data imported using `amanida_read` function w/o names checked by `check_names`
`comp.inf`	include compounds IDs from PubChem, InChIKey, SMILES, KEGG, ChEBI, HMDB, Drugbank, Molecular Mass and Molecular Formula

Details

Entries corresponding to metabolites are combined as follows:

- P-values are combined using Fisher method weighted by N and gamma distribution
- Fold-change are combined by weighted mean. Transformation works with fold-change transformed to log scale with base 2.

Vote-counting is computed based on votes. Punctuation of entries is based on trend, up-regulation gives 1, down-regulation give -1 and equal behavior gives 0. Total sum is divided then by the total number of entries on each compound.

Value

METAtable S4 object with p-value combined, fold-change combined and vote-counting for each compound

Examples

```
## Not run:
data("sample_data")

compute_amanida(sample_data)

## End(Not run)
```

`explore_plot` *Plot for compounds divergence in reports*

Description

`explore_plot` creates a bar-plot showing the votes divided in up-regulated and down-regulated and the global result for each compound.

Usage

```
explore_plot(data, type = "all", counts = NULL)
```

Arguments

`data`	an tibble obtained by `amanida_read` w/o names checked by `check_names`
`type`	select the subset of data to plot. Options are: • "all": all data will be displayed • "sub": only data over counts value will be displayed. Need counts value. • "mix": will display data over count value and elements with reports in both trends.Need counts value.
`counts`	value of vote-counting cut-off. Will be only displayed data over the cut-off.

Details

Sum of votes divided by trend are plotted, then is obtained the total result by compound summing both trends.

Value

a ggplot bar-plot showing the sum of votes for each compound divided by the trend

Examples

```
data("sample_data")

explore_plot(sample_data, type = "mix", counts = 1)
```

`getsampleDB` *Function to sample data path*

Description

Function to sample data path

Usage

```
getsampleDB()
```

`METAtables-class` *An S4 class to return results from* `compute_amanida` *or* `amanida_vote` *function*

Description

An S4 class to return results from `compute_amanida` or `amanida_vote` function

Slots

`stat` results for statistics combining p-values and fold-changes

`vote` vote-counting for metabolites

`sample_data` *Example input data for the amanida function*

Description

A dataset containing results from meta-analysis of metabolomic studies

Usage

```
sample_data
```

Format

A data frame with 143 rows and 6 variables:

id Name of the compound under study

pvalue P-value

foldchange Fold-change

N Number of samples of the compound

ref References

trend Trend: 1 (up), -1 (down) or 0 (none)

`volcano_plot` *Volcano plot of combined results*

Description

`volcano_plot` returns a volcano plot of the combined results on each metabolite obtained by `compute_amanida` function

Usage

```
volcano_plot(mets, cutoff = NULL)
```

Arguments

`mets`	an S4 METAtables object
`cutoff`	values for p-value and fold-change significance

Details

Results are presented as -log10 for p-value and log2 for fold-change. Values over the cut off are labeled. If not cutoff is provided will be used alpha 0.05 for p-value and 1.5 for logarithmic fold-change.

Value

plot of results

Examples

```
## Not run:
   data("sample_data")

   amanida_result <- compute_amanida(sample_data)
   volcano_plot(amanida_result)

## End(Not run)
```

`vote_plot` *Bar-plot for compounds vote-counting*

Description

`vote_plot` creates a bar-plot showing the vote-count for each compound.

Usage

```
vote_plot(mets, counts = NULL)
```

Arguments

`mets`	an S4 METAtables object obtained by `compute_amanida` or `amanida_vote`.
`counts`	value of vote-counting cut-off. Will be only displayed data over the cut-off.

Details

Vote-couting is the sum of number of reports up-regulated and the substraction of reports down-regulated.

Value

a ggplot bar-plot showing the vote-count per compound

Examples

```
## Not run:
    data("sample_data")
    result <- compute_amanida(sample_data)
    vote_plot(result)

## End(Not run)
```

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