

Package ‘famat’

February 27, 2021

Title Functional analysis of metabolic and transcriptomic data

Version 1.0.0

Description Famat is made to collect data about lists of genes and metabolites provided by user, and to visualize it through a Shiny app.

Information collected is:

- Pathways containing some of the user's genes and metabolites (obtained using a pathway enrichment analysis).
- Direct interactions between user's elements inside pathways.
- Information about elements (their identifiers and descriptions).
- Go terms enrichment analysis performed on user's genes.

The Shiny app is composed of:

- information about genes, metabolites, and direct interactions between them inside pathways.
- an heatmap showing which elements from the list are in pathways (pathways are structured in hierarchies).
- hierarchies of enriched go terms using Molecular Function and Biological Process.

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LazyData false

Depends R (>= 4.0)

Imports KEGGREST, MPINet, dplyr, gprofiler2, rWikiPathways, reactome.db, stringr, GO.db, ontologyIndex, tidyr, shiny, shinydashboard, shinyBS, plotly, magrittr, DT, clusterProfiler, org.Hs.eg.db

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compl_data

Data preparation for Shiny interface

Description

Complete and prepare data obtained with interactions function, to use it in the Shiny interface. GO terms enrichment analysis is performed using clusterProfiler.

Usage

```
compl_data(listparam)
```

Arguments

listparam Output from interactions function

Value

A list containing :

heatmap	Dataframe heatmap-like, with in abscissa elements of pathways ("X" is written if an element is present in a pathway), and with in ordinate hierarchies of pathways
meta_list	User's metabolites given in path_enrich function
allResBP	Results of Go BP terms enrichment analysis performed by clusterProfileR (20 best)
go_genelist	Dataframe containing enriched GO terms per genes of user's list

allResMF	Results of Go MF terms enrichment analysis performed by clusterProfileR (20 best)
types	Dataframe containing categories of pathways per pathways
genetype	List of genes categories, containing genes of user's list
metatab	Dataframe of metabolites and informations about them, as names and chebi ids
genetab	Dataframe of genes and informations about them, as gene symbols and names
intetab	Dataframe of direct interactions between elements of user's list, and informations about them as elements in the interaction, how they interact, and which pathways are concerned
gomf_tab	Dataframe of Go MF terms hierarchies containing our enriched GO terms, plus description of these GO terms and genes of user's list concerned by enriched GO terms
gobp_tab	Dataframe of Go BP terms hierarchies containing our enriched GO terms, plus description of these GO terms and genes of user's list concerned by enriched GO terms
gene_list	User's genes given in path_enrich function
gomflist	List containing GO MF terms hierarchies, with indices in the joliMF dataframe and genes concerned by the hierarchie
gobplis	List containing GO BP terms hierarchies, with indices in the joliMF dataframe and genes concerned by the hierarchy
hierabrite	List of pathways categories, containing pathways concerned by a category and their indices in "trait" dataframe
hierapath	List of hierarchies of pathways, containing indices of pathways in "trait" dataframe and elements contained in the hierarchy.
save_cluster_elem	Vector of clustered elements
centrality	Matrix trait-like with values of centralities (number of direct interactions between an element of user's list and other elements of the pathway) instead of "X"
inter_values	Matrix trait-like with values representing direct interactions (3/2/1, respectively for genes/metabolites implicated in a direct interaction, and for elements not implicated in a direct interaction) instead of "X"
gene_notin	Dataframe of genes which aren't in pathways and informations about them, as gene symbols and names
sub	Matrix trait-like with pathway and element informations instead of "X"

This list is used by rshiny function.

Author(s)

Emilie Secherre <emisecherre@gmail.com>

References

Guangchuang Yu, Li-Gen Wang, Yanyan Han and Qing-Yu He. clusterProfiler: an R package for comparing biological themes among gene clusters. *OMICS: A Journal of Integrative Biology* 2012, 16(5):284-287

See Also

[interactions rshiny](#)

Examples

```
## load example data
data(interactions_result)

compl_data_result=compl_data(interactions_result)
```

compl_data_result *Output of compl_data function*

Description

Enriched and structured informations about genes, metabolites, their interactions, pathways and enriched GO terms.

Usage

```
data("compl_data_result")
```

Format

List of 22 items.

heatmap Dataframe heatmap-like, with in abscissa elements of pathways ("X" is written if an element is present in a pathway), and with in ordinate hierarchies of pathways. A data frame with 16 rows and 9 variables.

path_name Hierarchies of pathways obtained by pathways enrichment analysis. Pathways are given by their name.

path_id Identifiers of pathways in hierarchies.

meta_ratio Metabolites ratio, so the part of user's metabolites in the total number of metabolites in the pathway.

gene_ratio Genes ratio, so the part of user's genes in the total number of genes in the pathway.

blank Just an empty column to separate heatmap data from pathways data (NA).

SLC6A12 The value "1" shows that the element SLC6A12 is in the pathway on the row, "0" shows it is not in this pathway (0–1).

Betaine The value "1" shows that the element Betaine is in the pathway on the row, "0" shows it is not in this pathway (0–1).

ATP The value "1" shows that the element ATP is in the pathway on the row, "0" shows it is not in this pathway (0–1).

Betaine / SLC6A12 The value "1" shows that the interaction Betaine / SLC6A12 is in the pathway on the row, "0" shows it is not in this pathway (0–1).

meta_list Vector containing user's metabolites (C00002, C00719)

allResBP Results of Go BP terms enrichment analysis performed by clusterProfileR (20 best). A data frame with 20 rows and 9 variables.

ID Identifiers of enriched GO terms.

Description Names of enriched GO terms.

- GeneRatio** Number of user's genes concerned by the enriched GO term, by total number of user's genes.
- BgRatio** Number of genes concerned by the enriched GO term, by the total number of annotated genes in the database.
- pvalue** Pvalue of the go term enrichment analysis (0.001392161–0.011536208).
- p.adjust** Adjusted pvalue of the go term enrichment analysis (0.01713291–0.02670275).
- qvalue** Qvalue of the go term enrichment analysis (0.001803464–0.002810816).
- geneID** Entrez Gene identifiers of all genes concerned by the enriched GO term (30, 6539).
- Count** Number of genes concerned by the enriched GO term described by an Entrez Gene identifier(1).
- go_genelist** Dataframe containing enriched GO terms per genes of user's list. A data frame with 13 rows and 2 variables.
- hgnc_symbol** Gene symbol of the gene concerned by an enriched GO term (SLC6A12, ACAA1).
- go_id** Identifier of the GO term concerning the gene (GO:0005328, GO:0015293, GO:0003333, GO:0015812, GO:0015171, GO:0042165, GO:0008028, GO:0006635, GO:0006625, GO:0033540, GO:0036109, GO:0008206, GO:0000038)
- allResMF** Results of Go MF terms enrichment analysis performed by clusterProfileR (20 best) A data frame with 20 rows and 9 variables.
- ID** Identifiers of enriched GO terms.
- Description** Names of enriched GO terms.
- GeneRatio** Number of user's genes concerned by the enriched GO term, by total number of user's genes.
- BgRatio** Number of genes concerned by the enriched GO term, by the total number of annotated genes in the database.
- pvalue** Pvalue of the go term enrichment analysis (0.001392161–0.011536208).
- p.adjust** Adjusted pvalue of the go term enrichment analysis (0.01713291–0.02670275).
- qvalue** Qvalue of the go term enrichment analysis (0.001803464–0.002810816).
- geneID** Entrez Gene identifiers of all genes concerned by the enriched GO term (30, 6539).
- Count** Number of genes concerned by the enriched GO term described by an Entrez Gene identifier(1).
- types** Dataframe containing categories of pathways per pathways. A data frame with 12 rows and 2 variables.
- id** Identifier of pathways from pathways enrichment analysis.
- root** Name of the pathway category concerning a pathway.
- genetype** List of genes categories, containing genes of user's list. A list of 3 items.
- metatab** Dataframe of metabolites and informations about them, as names and chebi ids. A data frame with 2 rows and 2 variables.
- id** Name of user's metabolites (ATP, Betaine).
- name** Chebi identifier of user's metabolites (CHEBI:15422, CHEBI:17750).
- genetab** Dataframe of genes and informations about them, as gene symbols and names. A data frame with 1 rows and 2 variables.
- id** Gene symbols of user's genes contained in pathways (SLC6A12).
- name** Name of user's genes contained in pathways (solute carrier family 6 member 12).
- intetab** Dataframe of direct interactions between elements of user's list, and informations about them as elements in the interaction, how they interact, and which pathways are concerned A data frame with 1 row and 8 variables.

- tag** Summary of elements concerned by the interaction (Betaine / SLC6A12)
- first_item** First element of the direct interaction (Betaine)
- link** Description of how the two elements interact (Control(In: ACTIVATION of BiochemicalReaction), controls-transport-of-chemical).
- sec_item** Second element of the direct interaction (SLC6A12)
- go** Value "1" means that a gene of the interaction is concerned by an enriched GO term, "0" means no element is concerned by an enriched GO term (1).
- path** Pathways containing the direct interaction ("R-HSA-112310, R-HSA-112315, R-HSA-112316, R-HSA-382551, R-HSA-425366, R-HSA-425393, R-HSA-425407, R-HSA-888590, R-HSA-352230, R-HSA-442660, R-HSA-888593")
- type** Interaction type, can be gene/gene, metabolite/metabolite, or gene/metabolite (g/m)
- cat** Categories of pathways containing the direct interaction (Neuronal System, Transport of small molecules)
- gomf_tab** Dataframe of Go MF terms hierarchies containing our enriched GO terms, plus description of these GO terms and genes of user's list concerned by enriched GO terms. A data frame with 93 rows and 3 variables.
- goterm** Hierarchies of enriched GO terms.
- go_name** Names of GO terms.
- genes** Genes concerned by GO terms.
- gobp_tab** Dataframe of Go BP terms hierarchies containing our enriched GO terms, plus description of these GO terms and genes of user's list concerned by enriched GO terms. A data frame with 107 rows and 3 variables.
- goterm** Hierarchies of enriched GO terms.
- go_name** Names of GO terms.
- genes** Genes concerned by GO terms.
- gene_list** Vector containing user's genes (ACAA1, SLC6A12)
- gomflist** List containing GO MF terms hierarchies, with indices in the joliMF dataframe and genes concerned by the hierarchy. A list of 3 items.
- gobplist** List containing GO BP terms hierarchies, with indices in the joliMF dataframe and genes concerned by the hierarchy. A list of 5 items.
- hierabrite** List of pathways categories, containing pathways concerned by a category and their indices in "trait" dataframe. A list of 3 items.
- hierapath** List of hierarchies of pathways, containing indices of pathways in "trait" dataframe and elements contained in the hierarchy. A list of 3 items.
- save_cluster_elem** Vector of clustered elements
- centrality** Matrix heatmap-like with values of centralities (number of direct interactions between an element of user's list and other elements of the pathway) instead of "X". Other cells contain the value "0" (0–65). An integer matrix with 16 rows and 9 columns.
- inter_values** Matrix heatmap-like with values representing direct interactions (3/2/1, respectively for genes/metabolites implicated in a direct interaction, and for elements not implicated in a direct interaction) instead of "X". Other cells contain the value "0" (0–3). An integer matrix with 16 rows and 9 columns.
- gene_notin** Dataframe of genes which aren't in pathways and informations about them, as gene symbols and names. A data frame with 1 row and 2 variables.
- id** Gene symbols of genes (ACAA1).
- name** Names of genes (acetyl-CoA acyltransferase 1).
- sub** Matrix heatmap-like with pathway and element informations instead of "X". Cells with no informations contain only "". A character matrix with 16 rows and 9 columns.

Source

compl_data function

genes	<i>List of genes.</i>
-------	-----------------------

Description

Example of a list of genes that can be provided by an user.

Usage

```
data("genes")
```

Format

A vector with 2 observations (ACAA1, SLC6A12).

Source

Sample of data from a study on chickens, under heat-stress condition.

interactions	<i>Interactions between genes and metabolites</i>
--------------	---

Description

Gather informations about direct interactions between genes and metabolites inside a pathway, and about pathways themselves. These informations are direct interactions between these two elements and number of relations between an element from the list provided by the user and other elements of the pathway (centrality). Direct interactions extraction was performed using BioPax, KGML and GPML files parsed with PaxtoolsR, graphite and author's parsers.

Usage

```
interactions(listk, listr, listw)
```

Arguments

listk	Output from path_enrich function, with "KEGG" argument.
listr	Output from path_enrich function, with "REAC" argument.
listw	Output from path_enrich function, with "WP" argument.

Value

A list containing :

size	Dataframe containing pathways, genes and metabolites in pathways (from the list or not), and number of elements in pathways
pathtot	Dataframe containing pathways names and ids from pathway enrichment analysis on Reactome, Kegg and Wikipathways pathways
tagged	Dataframe containing direct interactions between elements from the user's list per pathways
keggchebiname	Dataframe containing all human metabolites ids (kegg and chebi) and names
central	List of pathways, each pathway containing the number of direct interactions between an element of user's list and other elements in the pathway
no_path	Dataframe containing direct interactions between elements from the user's list, but not per pathways
genes	User's genes given in path_enrich function
meta	User's metabolites given in path_enrich function

This list is used by `compl_data` function.

Author(s)

Emilie Secherre <emisecherre@gmail.com>

References

Luna, A., Babur, O., Aksoy, A. B, Demir, E., Sander, C. (2015). "PaxtoolsR: Pathway Analysis in R Using Pathway Commons." *Bioinformatics*.

Sales G, Calura E, Cavalieri D, Romualdi C (2012). "graphite - a Bioconductor package to convert pathway topology to gene network." *BMC Bioinformatics*. <https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-13-20>.

See Also

[path_enrich](#) [compl_data](#)

Examples

```
## load example data
data(listk)
data(listr)
data(listw)

interactions_result=interactions(listk,listr,listw)
```

interactions_result *Output of interactions function*

Description

List containing informations about interactions between genes and metabolites, centrality and pathways. Direct interactions extraction was performed using BioPax, KGML and GPML files parsed with PaxtoolsR, graphite and author's parsers.

Usage

```
data("interactions_result")
```

Format

List of 8 items.

size Description on which elements (from user's list or not) are contained in pathways from pathway enrichment analysis. A data frame with 286 rows and 9 variables.

path Pathways obtained through pathways enrichment analysis on KEGG, Reactome and Wikipathways pathways.

nb_gene_query Number of user's genes contained in the pathway (0–2).

gene_que User's genes contained in the pathway (ACAA1, SLC6A12, ACAA1 # SLC6A12).

nb_gene_tot Total number of genes contained in the pathway (0–2075).

genes All the genes contained in the pathway.

nb_meta_query Number of user's metabolites contained in the pathway (0–2).

meta_que User's metabolites contained in the pathway (Betaine, ATP, Betaine # ATP, ATP # Betaine).

nb_meta_tot Total number of metabolites contained in the pathway (0–915).

meta All the metabolites contained in the pathway.

pathtot All results of pathways enrichment analysis performed on Kegg, Reactome and Wikipathways pathways. A data frame with 286 rows and 2 variables.

name Name of pathways resulting in genes pathway enrichment analysis performed on Kegg, Reactome and Wikipathways.

id Identifiers of pathways resulting in genes pathway enrichment analysis performed on Kegg, Reactome and Wikipathways.

tagged Description of all direct interactions between user's elements in pathways. A data frame with 11 rows and 6 variables.

from First element of the direct interaction (Betaine, SLC6A12)

link Description of how the two elements interact (Control(In: ACTIVATION of BiochemicalReaction), controls-transport-of-chemical).

to Second element of the direct interaction (Betaine, SLC6A12)

path Pathway containing the direct interaction (R-HSA-112310, R-HSA-112315, R-HSA-112316, R-HSA-382551, R-HSA-425366, R-HSA-425393, R-HSA-425407, R-HSA-888590, R-HSA-352230, R-HSA-442660, R-HSA-888593)

tag Summary of elements concerned by the interaction (Betaine / SLC6A12, SLC6A12 / Betaine)

- type** Interaction type, can be gene/gene, metabolite/metabolite, or gene/metabolite (g/m)
- keggchebiname** Dataframe containing all human metabolites ids (kegg and chebi) and names. A data frame with 16075 rows and 3 variables.
- kegg** Kegg_compound identifiers of all human metabolites.
- chebi** Chebi identifiers of all human metabolites.
- name** Names of all human metabolites.
- central** List of pathways, each pathway containing the number of direct interactions between an element of user's list and other elements in the pathway. A list of 138 items.
- no_path** Dataframe containing direct interactions between elements from the user's list, but not per pathways. A data frame with 1 rows and 6 variables.
- from** First element of the direct interaction (Betaine, SLC6A12)
- link** Description of how the two elements interact (Control(In: ACTIVATION of BiochemicalReaction), controls-transport-of-chemical).
- to** Second element of the direct interaction (Betaine, SLC6A12)
- path** Pathways containing the direct interaction ("R-HSA-112310, R-HSA-112315, R-HSA-112316, R-HSA-382551, R-HSA-425366, R-HSA-425393, R-HSA-425407, R-HSA-888590, R-HSA-352230, R-HSA-442660, R-HSA-888593")
- tag** Summary of elements concerned by the interaction (Betaine / SLC6A12)
- type** Interaction type, can be gene/gene, metabolite/metabolite, or gene/metabolite (g/m)
- genes** Vector containing user's genes (ACAA1, SLC6A12)
- meta** Vector containing user's metabolites (C00002, C00719)

Source

interactions function.

References

Luna, A., Babur, O., Aksoy, A. B, Demir, E., Sander, C. (2015). "PaxtoolsR: Pathway Analysis in R Using Pathway Commons." *Bioinformatics*.

Sales G, Calura E, Cavalieri D, Romualdi C (2012). "graphite - a Bioconductor package to convert pathway topology to gene network." *BMC Bioinformatics*. <https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-13-20>.

listk

Pathway enrichment analysis results for KEGG pathways.

Description

Results of pathways enrichment analysis on the list of genes and metabolites, using KEGG pathways. Pathways enrichment analysis is performed using MPINet for metabolites and gprofiler2 for genes.

Usage

```
data("listk")
```

Format

A list of 4 items.

resmeta Pathway enrichment analysis results for metabolites. A data frame with 7 rows and 2 variables.

name Name of pathways resulting in metabolites pathway enrichment analysis.

id Identifiers of pathways resulting in metabolites pathway enrichment analysis.

resgene Pathway enrichment analysis results for genes. A data frame with 11 rows and 2 variables.

name Name of pathways resulting in genes pathway enrichment analysis.

id Identifiers of pathways resulting in genes pathway enrichment analysis.

gened Vector containing user's genes (ACAA1, SLC6A12)

metad Vector containing user's metabolites (C00002, C00719)

Source

path_enrich function.

References

Yanjun Xu, Chunquan Li and Xia Li (2013). MPINet: The package can implement the network-based metabolite pathway identification of pathways.. R package version 1.0. <https://CRAN.R-project.org/package=MPINet>

Liis Kolberg and Uku Raudvere (2020). gprofiler2: Interface to the 'g:Profiler' Toolset. R package version 0.2.0. <https://CRAN.R-project.org/package=gprofiler2>

listr

Pathway enrichment analysis results for Reactome pathways.

Description

Results of pathways enrichment analysis on the list of genes and metabolites, using Reactome pathways. Pathways enrichment analysis is performed using MPINet for metabolites and gprofiler2 for genes.

Usage

```
data("listr")
```

Format

A list of 4 items.

resmeta Pathway enrichment analysis results for metabolites. A data frame with 278 rows and 2 variables.

name Name of pathways resulting in metabolites pathway enrichment analysis.

id Identifiers of pathways resulting in metabolites pathway enrichment analysis.

resgene Pathway enrichment analysis results for genes. A data frame with 27 rows and 2 variables.

name Name of pathways resulting in genes pathway enrichment analysis.

id Identifiers of pathways resulting in genes pathway enrichment analysis.

gened Vector containing user's genes (ACAA1, SLC6A12)

metad Vector containing user's metabolites (C00002, C00719)

Source

path_enrich function.

References

Yanjun Xu, Chunquan Li and Xia Li (2013). MPINet: The package can implement the network-based metabolite pathway identification of pathways.. R package version 1.0. <https://CRAN.R-project.org/package=MPINet>

Liis Kolberg and Uku Raudvere (2020). gprofiler2: Interface to the 'g:Profiler' Toolset. R package version 0.2.0. <https://CRAN.R-project.org/package=gprofiler2>

listw

Pathway enrichment analysis results for Wikipathways pathways.

Description

Results of pathways enrichment analysis on the list of genes and metabolites, using Wikipathways pathways. Pathways enrichment analysis is performed using MPINet for metabolites and gprofiler2 for genes.

Usage

```
data("listw")
```

Format

A list of 4 items.

resmeta Pathway enrichment analysis results for metabolites. A data frame with 48 rows and 2 variables.

name Name of pathways resulting in metabolites pathway enrichment analysis.

id Identifiers of pathways resulting in metabolites pathway enrichment analysis.

resgene Pathway enrichment analysis results for genes. A data frame with 8 rows and 2 variables.

name Name of pathways resulting in genes pathway enrichment analysis.

id Identifiers of pathways resulting in genes pathway enrichment analysis.

gened Vector containing user's genes (ACAA1, SLC6A12)

metad Vector containing user's metabolites (C00002, C00719)

Source

path_enrich function.

References

Yanjun Xu, Chunquan Li and Xia Li (2013). MPINet: The package can implement the network-based metabolite pathway identification of pathways.. R package version 1.0. <https://CRAN.R-project.org/package=MPINet>

Liis Kolberg and Uku Raudvere (2020). gprofiler2: Interface to the 'g:Profiler' Toolset. R package version 0.2.0. <https://CRAN.R-project.org/package=gprofiler2>

meta	<i>List of metabolites.</i>
------	-----------------------------

Description

Example of a list of metabolites that can be provided by an user.

Usage

```
data("meta")
```

Format

A vector with 2 observations (C00002, C00719).

Source

Sample of data from a study on chickens, under heat-stress condition.

path_enrich	<i>Pathway enrichment analysis</i>
-------------	------------------------------------

Description

Perform a pathway enrichment analysis using a list of genes and a list of metabolites. Pathways enrichment analysis is performed using MPINet for metabolites and gprofiler2 for genes.

Usage

```
path_enrich(source, metabo, genes)
```

Arguments

source	Pathways database used, either Kegg ("KEGG"), Reactome ("REAC") or Wikipathays ("WP")
metabo	Dataframe with three columns : the first column contain the list of metabolites, the second some quantitative data about the metabolites, the last one words "DOWN" or "UP" depending on the metabolites concentration behavior in a certain condition. Last two columns can contain only/some NAs. All metabolites ids are KEGG Compound ids.
genes	Dataframe with three columns : the first column contain the list of genes, the second some quantitative data about the genes, the last one words "DOWN" or "UP" depending on the genes expression behavior in a certain condition. Last two columns can contain only/some NAs. All genes ids are gene symbol.

Value

A list containing :

resmeta	Results of metabolites pathway enrichment analysis
resgene	Results of genes pathway enrichment analysis
genes	Vector containing genes
metabo	Vector containing metabolites

This list is used by `interactions` function.

Author(s)

Emilie Secherre <emisecherre@gmail.com>

References

Yanjun Xu, Chunquan Li and Xia Li (2013). MPINet: The package can implement the network-based metabolite pathway identification of pathways.. R package version 1.0. <https://CRAN.R-project.org/package=MPINet>

Liis Kolberg and Uku Raudvere (2020). gprofiler2: Interface to the 'g:Profiler' Toolset. R package version 0.2.0. <https://CRAN.R-project.org/package=gprofiler2>

See Also

[interactions](#)

Examples

```
## load example data
data(genes)
data(meta)

## perform pathway enrichment analysis on Reactome pathways
listr=path_enrich("REAC", meta, genes)
```

rshiny

Shiny interface

Description

Visualize and filter all fonctionnal informations gathered by famat using a Shiny interface.

Usage

```
rshiny(listdata)
```

Arguments

listdata Output from `compl_data` function

Value

Shiny interface

Author(s)

Emilie Secherre <emisecherre@gmail.com>

References

Winston Chang, Joe Cheng, JJ Allaire, Yihui Xie and Jonathan McPherson (2020). shiny: Web Application Framework for R. R package version 1.5.0. <https://CRAN.R-project.org/package=shiny>

See Also

[compl_data](#)

Examples

```
## load example data
data(compl_data_result)

## Not run: rshiny(compl_data_result)
```

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