Package 'graphite'

July 9, 2025

```
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Description Graph objects from pathway topology derived from KEGG, Panther,
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BugReports https://github.com/sales-lab/graphite/issues
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```

Version 1.54.0

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 $as. \verb|list.Pathway| Lists into lists.$

Description

Converts a PathwayList into a list of Pathways.

Usage

```
## S3 method for class 'PathwayList' as.list(x, ...)
```

Arguments

x a PathwayList object ... extra arguments to as.list

Value

A list of pathways.

Author(s)

Gabriele Sales

See Also

 ${\tt PathwayList}$

```
as.list(pathways("hsapiens", "kegg"))
```

buildPathway 3

Description

This function creates a new object of type Pathway given a data frame describing its edges.

Usage

Arguments

id the pathway identifier.title the title of the pathway.

species the species the pathway belongs to.

database the name of the database the pathway derives from.

proteinEdges a data.frame of edges between proteins (or genes).

Must have the following columns: src_type, src, dest_type, dest, direction and

type.

Direction must be one of the two strings: "directed" or "undirected".

metaboliteEdges

interactions between metabolites.

Can be NULL. Otherwise, it must have the same structure as proteinEdges.

mixedEdges interactions between metabolites and proteins.

Can be NULL. Otherwise, it must have the same structure as proteinEdges.

timestamp when the pathway was annotated, by default the time buildPathway is called.

Value

A new Pathway instance.

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```
mixed <- data.frame(src_type = "CHEBI", src="77750",</pre>
                     dest_type = "ENTREZID", dest="7157",
                     direction="undirected", type="binding")
pathway <- buildPathway("#1", "example", "hsapiens", "database",</pre>
                         edges, mixedEdges = mixed)
```

convertIdentifiers

Convert the node identifiers of a pathway.

Description

Converts the node identifiers of pathways.

If the option Ncpus is set to a value larger than 1 and the package parallel is installed, the conversion procedure will automatically use multiple cores.

Usage

```
convertIdentifiers(x, to)
```

Arguments

can be a list of pathways or a single pathway Χ

a string describing the type of the identifier. Can assume the values "entrez", to "symbol" or the name of one of the columns provided by an Annotation package

(for example, "UNIPROT").

Value

A Pathway object.

See Also

Pathway

```
r <- pathways("hsapiens", "reactome")</pre>
convertIdentifiers(r$`mTORC1-mediated signalling`, "symbol")
```

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cytoscapePlot

Plot a pathway graph in Cytoscape

Description

Renders the topology of a pathway as a Cytoscape graph.

Usage

```
cytoscapePlot(pathway, ..., cy.ver = 3)
```

Arguments

pathway a Pathway object.

... optional arguments forwarded to pathwayGraph.

cy.ver select a Cytoscape version. Only version 3 is supported in this release.

Details

Requires the RCy3 package.

Value

An invisible list with two items:

graph the graphNEL object sent to Cytoscape.

suid the RCy3 network SUID.

See Also

```
Pathway
```

pathwayGraph

```
## Not run:
    r <- pathways()
    cytoscapePlot(convertIdentifiers(reactome$`Unwinding of DNA`, "symbol"))
## End(Not run)</pre>
```

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Pathway-class

Class "Pathway"

Description

A biological pathway.

Variants

A Pathway instance actually stores multiple variants of the same biological data.

This is the list of included variants:

- proteins: includes only interactions among proteins;
- metabolites: includes only interactions among metabolites;
- mixed: includes all available interactions.

Methods

```
pathwayId(p): Returns the native ID of the pathway.
pathwayTitle(p): Returns the title of the pathway.
pathwayDatabase(p): Returns the name of the database the pathway was derived from.
pathwaySpecies(p): Returns the name of the species in which the pathway was annotated.
pathwayTimestamp(p): Returns the date of pathway data retrieval.
pathwayURL(p): Returns the URL of the pathway in its original database, if available.
convertIdentifiers(p, to): Returns a new pathway using a different type of node identifiers.
edges(p, which = c("proteins", "metabolites", "mixed"), stringsAsFactors = TRUE): Returns
    a data.frame describing the edges of this pathway.
    The option which selects the desired pathway variant (see section "Variants" above).
    If stringsAsFactors is TRUE, strings are converted to factors.
nodes(p, which = c("proteins", "metabolites", "mixed")): Returns the names of the nodes
    belonging to this pathway.
    The option which selects the desired pathway variant (see section "Variants" above).
plot(p): Shows the pathway topology in Cytoscape.
runClipper(p, expr, classes, method, ...): Runs a clipper analysis over the pathway.
runTopologyGSA(p, test, exp1, exp2, alpha, ...): Runs a topologyGSA analysis over the path-
    way.
```

Author(s)

Gabriele Sales

See Also

pathways

pathwayDatabases 7

Examples

```
reactome <- pathways("hsapiens", "reactome")
pathway <- reactome[[1]]

pathwayTitle(pathway)
pathwaySpecies(pathway)
nodes(pathway)
edges(pathway)</pre>
```

pathwayDatabases

List the available pathway databases.

Description

Obtains the list of pathway databases available through graphite.

Usage

```
pathwayDatabases()
```

Value

Returns a data. frame with two columns: species and database.

Author(s)

Gabriele Sales

See Also

pathways

```
pathwayDatabases()
```

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pathwayGraph

Graph representing the topology of a pathway

Description

Builds a graphNEL object representing the topology of a pathway.

Usage

```
pathwayGraph(pathway, which = "proteins", edge.types = NULL)
```

Arguments

pathway a Pathway object.

which the pathway variant you want.

See Pathway documentation for a list of the supported variants.

edge. types keep only the edges maching the type names in this vector.

Value

A graphNEL object.

See Also

Pathway graphNEL

Examples

```
r <- pathways("hsapiens", "reactome")
pathwayGraph(r$`mTORC1-mediated signalling`, edge.types="Binding")</pre>
```

PathwayList-class

Class "PathwayList"

Description

A collection of pathways from a single database.

Extends

```
Class "Pathways", directly.
```

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Methods

1[i] returns a selection of the pathways contained in the pathway list.

1[[i]] gives access to one of the pathways contained in the pathway list.

1\$'title' loads a pathways by its title.

convertIdentifiers(1, to) returns a new list of pathways using a different type of node identifiers

length(1) returns the number of pathways contained in the list.

names(1) returns the titles of the pathways contained in the list.

prepareSPIA(1, pathwaySetName, print.names=FALSE) prepares the pathways for a SPIA analysis.

runClipper(1, expr, classes, method, maxNodes=150, ...) runs a clipper analysis over all the pathways in the list.

runTopologyGSA(1, test, exp1, exp2, alpha, maxNodes=150, ...) runs a topologyGSA analysis over all the pathways in the list.

Author(s)

Gabriele Sales

See Also

pathways

pathways

Retrieve a list of pathways.

Description

Retrieve a list of pathways from a database for a given species. graphite currently supports the following databases:

- KEGG
- PANTHER
- PathBank
- PharmGKB
- Reactome
- SMPDB
- WikiPathways

Call the pathwayDatabase function for more details.

Usage

```
pathways(species, database)
```

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Arguments

species one of the supported species

database the name of the pathway database

Value

A PathwayList object.

See Also

PathwayList, pathwayDatabases

Examples

```
pathways("hsapiens", "reactome")
```

Pathways-class

Class "Pathways"

Description

A virtual class acting as a common parent to all other classes representing pathway databases.

Objects from the Class

A virtual Class: No objects may be created from it.

Methods

No methods defined with class "Pathways" in the signature.

Author(s)

Gabriele Sales

See Also

 ${\tt PathwayList}$

prepareSPIA 11

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pre	par	eSP.	LΑ

Prepare pathway dataset needed by runSPIA.

Description

Prepare pathway dataset needed by runSPIA. See runSPIA and spia for more details.

Usage

```
prepareSPIA(db, pathwaySetName, print.names = FALSE)
```

Arguments

```
db a PathwayList object or a list of Pathways.

pathwaySetName name of the output pathway set.

print.names print pathway names as the conversion advances.
```

Value

This function has no return value.

References

Tarca AL, Draghici S, Khatri P, Hassan SS, Mittal P, Kim JS, Kim CJ, Kusanovic JP, Romero R. A novel signaling pathway impact analysis. Bioinformatics. 2009 Jan 1;25(1):75-82.

Adi L. Tarca, Sorin Draghici, Purvesh Khatri, et. al, A Signaling Pathway Impact Analysis for Microarray Experiments, 2008, Bioinformatics, 2009, 25(1):75-82.

Draghici, S., Khatri, P., Tarca, A.L., Amin, K., Done, A., Voichita, C., Georgescu, C., Romero, R.: A systems biology approach for pathway level analysis. Genome Research, 17, 2007.

See Also

```
runSPIA
spia
PathwayList
```

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runSPIA	Run SPIA analysis	

Description

Run a topological analysis on an expression dataset using SPIA.

Usage

```
runSPIA(de, all, pathwaySetName, ...)
```

Arguments

de	A named vector containing log2 fold-changes of the differentially expressed genes. The names of this numeric vector are Entrez gene IDs.
all	A vector with the Entrez IDs in the reference set. If the data was obtained from a microarray experiment, this set will contain all genes present on the specific array used for the experiment. This vector should contain all names of the 'de' argument.
pathwaySetName	The name of a pathway set created with prepareSPIA.
	Additional options to pass to spia.

Details

The spia option "organism" is internally used. It is an error use it in the additional options.

Value

The same of spia, without KEGG links. A data frame containing the ranked pathways and various statistics: pSize is the number of genes on the pathway; NDE is the number of DE genes per pathway; tA is the observed total preturbation accumulation in the pathway; pNDE is the probability to observe at least NDE genes on the pathway using a hypergeometric model; pPERT is the probability to observe a total accumulation more extreme than tA only by chance; pG is the p-value obtained by combining pNDE and pPERT; pGFdr and pGFWER are the False Discovery Rate and respectively Bonferroni adjusted global p-values; and the Status gives the direction in which the pathway is perturbed (activated or inhibited).

References

Tarca AL, Draghici S, Khatri P, Hassan SS, Mittal P, Kim JS, Kim CJ, Kusanovic JP, Romero R. A novel signaling pathway impact analysis. Bioinformatics. 2009 Jan 1;25(1):75-82.

Adi L. Tarca, Sorin Draghici, Purvesh Khatri, et. al, A Signaling Pathway Impact Analysis for Microarray Experiments, 2008, Bioinformatics, 2009, 25(1):75-82.

Draghici, S., Khatri, P., Tarca, A.L., Amin, K., Done, A., Voichita, C., Georgescu, C., Romero, R.: A systems biology approach for pathway level analysis. Genome Research, 17, 2007.

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See Also

spia

Examples

```
if (require(SPIA) && require(hgu133plus2.db)) {
   data(colorectalcancer)

top$ENTREZ <- mapIds(hgu133plus2.db, top$ID, "ENTREZID", "PROBEID", multiVals = "first")
   top <- top[!is.na(top$ENTREZ) & !duplicated(top$ENTREZ), ]
   top$ENTREZ <- paste("ENTREZID", top$ENTREZ, sep = ":")
   tg1 <- top[top$adj.P.Val < 0.05, ]

DE_Colorectal = tg1$logFC
   names(DE_Colorectal) <- tg1$ENTREZ
   ALL_Colorectal <- top$ENTREZ

kegg <- pathways("hsapiens", "kegg")[1:20]
   kegg <- convertIdentifiers(kegg, "ENTREZID")
   prepareSPIA(kegg, "keggEx")
   runSPIA(de = DE_Colorectal, all = ALL_Colorectal, "keggEx")
   unlink("keggExSPIA.RData")
}</pre>
```

runTopologyGSA

Run a topological analysis on an expression dataset using topology GSA.

Description

Use graphical models to test the pathway components highlighting those involved in its deregulation.

If the option Ncpus is set to a value larger than 1 and the package parallel is installed, the conversion procedure will automatically use multiple cores.

Usage

```
runTopologyGSA(x, test, exp1, exp2, alpha, ...)
```

Arguments

Χ	a PathwayList, a list of Pathways or a single Pathway object.
test	Either "var" and "mean". Determine the type of test used by topologyGSA.
exp1	Experiment matrix of the first class, genes in columns.
exp2	Experiment matrix of the second class, genes in columns.
alpha	Significance level of the test.

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... Additional parameters forwarded to topologyGSA.

When invoked on a PathwayList, can use the named option "maxNodes" to

Details

This function produces a warning and returns NULL when the number of genes in common between the expression matrices and the pathway is less than 3.

limit the analysis to those pathways having up to this given number of nodes.

Value

See documentation of pathway.var.test and pathway.mean.test.

References

Massa MS, Chiogna M, Romualdi C. Gene set analysis exploiting the topology of a pathway. BMC System Biol. 2010 Sep 1;4:121.

```
if (require(topologyGSA)) {
   data(examples)
   colnames(y1) <- paste("SYMBOL", colnames(y1), sep = ":")
   colnames(y2) <- paste("SYMBOL", colnames(y2), sep = ":")

   k <- pathways("hsapiens", "kegg")
   p <- convertIdentifiers(k[["Fc epsilon RI signaling pathway"]], "SYMBOL")
   runTopologyGSA(p, "var", y1, y2, 0.05)
}</pre>
```

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