# **KEGGgraph**

October 25, 2011

KEGGEdge-class Class 'KEGGEdge'

### Description

A class to represent 'relation' elements in KGML files and edge objects in a KEGG graph

### **Objects from the Class**

Objects are normally created by parseRelation function, which is not intended to be called by user directly

#### Slots

entry1ID: The entryID of the first KEGGNode
entry2ID: The entryID of the second KEGGNode
type: The type of the relation, see getType-methods
subtype: The subtype(s) of the edge, a list of KEGGEdgeSubType

# Methods

```
getEntryID signature(obj = "KEGGEdge"): Get entryIDs of the edge in the order speci-
fied by the direction of the edge
```

getType signature(object = "KEGGEdge"): Get the relation type

show signature(object = "KEGGEdge"): Show method

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

# References

KGML Manual http://www.genome.jp/kegg/docs/xml/

#### See Also

KEGGNode-class

#### Examples

```
mapfile<- system.file("extdata/map00260.xml", package="KEGGgraph")
maptest <- parseKGML(mapfile)
x <- edges(maptest)[[1]]
class(x)
## examples to extract information from KEGGEdge
getName(x)
getEntryID(x)
getType(x)
getSubtype(x)
subtype <- getSubtype(x)[[1]]
getName(subtype)</pre>
```

KEGGEdgeSubType-class Class "KEGGEdgeSubType"

#### Description

A class to represent subtype in KEGG

# **Objects from the Class**

Objects can be created by calls of the form new ("KEGGEdgeSubType", ...).

# Slots

name: Object of class "character", name of the subtype
value: Object of class "character", value of the subtype

# Methods

```
getName signature(object = "KEGGEdgeSubType"): getting subtype name
getValue signature(object = "KEGGEdgeSubType"): getting subtype value
show signature(object = "KEGGEdgeSubType"): show method
```

#### Note

Please note that 'KEGGEdgeSubtype' is a data frame storing subtype predefinitions, the 'type' with lowercases. 'KEGGEdgeSubType' is however a class representing these subtypes.

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

### *KEGGEdgeSubtype*

### See Also

KEGGEdge-class

# Examples

```
showClass("KEGGEdgeSubType")
## use example(KEGGEdge-class) for more examples
```

KEGGEdgeSubtype Predefinitions of node or edge types

# Description

The KGML files define node and edge type and subtypes, which are summarized in these data frames.

# Usage

```
data(KEGGEdgeSubtype)
data(KEGGNodeType)
data(KEGGEdgeType)
```

#### Format

They are stored as data frames

# Details

They are used by graph render functions to identify different types of objects, user could use them to classify edges or nodes.

### References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

# Examples

```
data(KEGGEdgeSubtype)
data(KEGGEdgeType)
data(KEGGNodeType)
```

KEGGGraphics-class class 'KEGGGraphics'

#### Description

A class to represent 'graphics' element in KGML files

### **Objects from the Class**

This method is mainly used to extract visualization information from KGML files.

Objects can be created by calling parseGraphics

# Slots

name: Object of class "character" graphics name x: Object of class "integer" x coordinate in KEGG figure y: Object of class "integer" y coordinate in KEGG figure type: Object of class "character" graphics type (shape) width: Object of class "integer" witdh of the symbol height: Object of class "integer" height of the symbol fgcolor: Object of class "character" foreground color bgcolor: Object of class "character" background color

### Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

#### References

KGML Manual http://www.genome.jp/kegg/docs/xml/

### See Also

parseGraphics

# Examples

showClass("KEGGGraphics")

KEGGGroup-class Class "KEGGGroup"

# Description

Class to represent 'group' nodes in KEGG pathways

#### **Objects from the Class**

The objects are usually created by parseEntry function and is not intended to be called directly by users.

# Slots

component: Component of the group

entryID: see the slot of KEGGNode-class

graphics: see the slot of KEGGNode-class

link: see the slot of KEGGNode-class

map: see the slot of KEGGNode-class

name: see the slot of KEGGNode-class

reaction: see the slot of KEGGNode-class

type: see the slot of KEGGNode-class

# Extends

Class "KEGGNode", directly.

#### Methods

### Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

# See Also

KEGGNode-class

#### Examples

showClass("KEGGGroup")

KEGGNode-class Class "KEGGNode"

# Description

The class to present 'entry' element in KGML files and nodes in KEGG graphs

# **Objects from the Class**

Objects can be created by calls of the function parseEntry and is not intended to be directly created by users.

# Slots

- entryID: entryID, the 'id' attribute of 'entry' elements in KGML files. In each KGML file the entryID is specified by auto-increment integers, therefore entryIDs from two individual KGML files are not unique. However, if 'expandGenes' option is specified in KEGGpathway2Graph function, the unique KEGGID will replace the default integer as the new entryID, which is unique in biological context
- name: Name of the node
- type: Type of the node, use data (KEGGNodeType) to see available values
- link: URL link of the node
- reaction: Reaction of the node
- map: Map of the node

graphics: Graphic details (including display name) of the node, an object of KEGGGGraphics

### Methods

getDisplayName signature (object = "KEGGNode"): get display name

getEntryID signature(obj = "KEGGNode"): get entryID, in case of gene-expanded graphs
this is the same as getKEGGID

getKEGGID signature(object = "KEGGNode"): get KEGGID

getType signature (object = "KEGGNode"): get the type of the node

<-name signature(object = "KEGGNode"): replace name

getComponent signature(obj = "KEGGNode"): returns entryID(the same as getEntryID),
 for compatibility with KEGGGroup-class

show signature(object = "KEGGNode"): show method

#### Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

# References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

# See Also

KEGGEdge-class, parseEntry

#### KEGGPathway-class

#### Examples

```
## We show how to extract information from KEGGNode object
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)
ns <- nodes(pathway)
node <- ns[[1]]
show(node)
getName(node)
getDisplayName(node)
getEntryID(node)
getKEGGID(node)
```

KEGGPathway-class Class "KEGGPathway"

#### Description

A class to represent KEGG pathway

### **Objects from the Class**

Objects can be created by calls of the form new("KEGGPathway", ...) . Normally they are created by parseKGML.

### Slots

pathwayInfo: An object of KEGGPathwayInfo-class nodes: List of objects of KEGGNode-class edges: List of objects of KEGGEdge-class reactions: List of objects of KEGGReaction-class

# Methods

```
edges signature(object = "KEGGPathway", which = "ANY"): KEGGEdges of the
    pathway
edges<- signature(object = "KEGGPathway"): setting edges
edges</pre>
```

getName signature(object = "KEGGPathway"): getting pathway name
getTitle signature(object = "KEGGPathway"): getting pathway title
nodes<- signature(object = "KEGGPathway", value = "ANY"): setting nodes
nodes signature(object = "KEGGPathway"): KEGGNodes of the pathway
getPathwayInfo signature(object = "KEGGPathway"): getting KEGGPathwayInfo
getTitle signature(object = "KEGGPathway"): getting title of the pathway
show signature(object = "KEGGPathway"): display method</pre>

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

#### References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

#### See Also

parseKGML, KEGGEdge-class, KEGGNode-class, KEGGReaction-class

#### Examples

```
## We show how to extract information from KEGGPathway objects
## Parse KGML file into a 'KEGGPathway' object
mapfile <- system.file("extdata/map00260.xml", package="KEGGgraph")</pre>
maptest <- parseKGML(mapfile)</pre>
## short summary of the pathway
maptest
## get information of the pathway
getPathwayInfo(maptest)
## nodes of the pathway
nodes <- nodes(maptest)</pre>
node <- nodes[[3]]</pre>
getName(node)
getType(node)
getDisplayName(node)
## edges of the pathway
edges <- edges(maptest)
edge <- edges[[3]]</pre>
getEntryID (edge)
getSubtype (edge)
```

KEGGPathwayInfo-class Class "KEGGPathwayInfo"

# Description

A class to represent information of a KEGG pathway

# **Objects from the Class**

Objects can be created by calls of the function parsePathwayInfo.

# Slots

name: Object of class "character" Pathway name
org: Object of class "character" Organism
number: Object of class "character" Number
title: Object of class "character" Title of the pathway
image: Object of class "character" Image URL
link: Object of class "character" URL Link

#### **KEGGReaction-class**

#### Methods

```
getTitle signature(object = "KEGGPathwayInfo"): get title of the pathway
show signature(object = "KEGGPathwayInfo"): show method
```

### Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

# References

KGML Document Manual http://www.genome.jp/kegg/docs/xml/

### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)
pi <- getPathwayInfo(pathway)</pre>
```

class(pi)

getTitle(pi)

KEGGReaction-class Class "KEGGReaction"

#### Description

A class to present 'reaction' elements in KGML files

# **Objects from the Class**

Objects can be created by calls of the function parseReaction.

# Slots

```
name: Object of class "character" the KEGGID of this reaction, e.g. "rn:R02749"
```

type: Object of class "character" the type of this reaction, either 'reversible' or 'irreversible'

- substrateName: Object of class "character", KEGG identifier of the COMPOUND database
   or the GLYCAN database e.g. "cpd:C05378"
- substrateAltName: Object of class "character" alternative name of its parent substrate element

productName: Object of class "character" specifies the KEGGID of the product

productAltName: Object of class "character" alternative name of its parent product element

# Methods

```
show signature(object = "KEGGReaction"): show method
getName signature(object = "KEGGReaction"): get the KEGGID of the reaction
getType signature(object = "KEGGReaction"): get the type of the reaction
getSubstrate signature(object = "KEGGReaction"): get the name of substrate
getProduct signature(object = "KEGGReaction"): get the name of product
```

#### Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

#### References

KGML Document Manual http://www.genome.jp/kegg/docs/xml/

#### Examples

```
## We show how to extract reactions from a 'KEGGPathway' object
mapfile <- system.file("extdata/map00260.xml", package="KEGGgraph")
maptest <- parseKGML(mapfile)
mapReactions <- getReactions(maptest)
## More details about reaction
reaction <- mapReactions[[1]]
getName(reaction)
getType(reaction)
getProduct(reaction)
getProduct(reaction)</pre>
```

KEGGpathway2Graph Parses KEGGpathway to graph

#### Description

The function parses an object of KEGGPathway-class into graph.

### Usage

```
KEGGpathway2Graph(pathway, genesOnly = TRUE, expandGenes = TRUE)
```

# Arguments

pathway	An instance of KEGGPathway-class
genesOnly	logical, should only the genes are maintained and other types of nodes (compounds, etc) neglected? TRUE by default
expandGenes	logical, should homologue proteins expanded? TRUE by default

#### Details

When 'expandGenes=TRUE', the nodes have unique names of KEGGID (in the form of 'org:xxxx', for example 'hsa:1432'), otherwise an auto-increment index given by KEGG is used as node names. In the latter case, the node names are duplicated and graphs cannot be simply merged before the nodes are unique.

KEGG node and edge data is stored in 'nodeData' and 'edgeData' slots respectively, which can be extracted by getKEGGnodeData and getKEGGedgeData.

# Value

A directed graph.

#### KEGGpathway2reactionGraph

#### Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

### See Also

parseKGML2Graph

### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
kegg.pathway <- parseKGML(sfile)
gR.compact<- KEGGpathway2Graph(kegg.pathway,expandGenes=FALSE)</pre>
```

```
KEGGpathway2reactionGraph
```

Convert chemical reaction network of KEGG pathway into graph

### Description

Regulatory pathways are always viewed as protein networks, so there is no 'reaction' information saved in their KGML files. Metabolic pathways are viewed both as both protein networks and chemical networks, hence the KEGGPathway-class object may have reactions information among chemical compounds.

This functions extracts reaction information from KEGG pathway, and convert the chemical compound reaction network into directed graph.

### Usage

```
KEGGpathway2reactionGraph(pathway, uniqueReaction = TRUE)
```

### Arguments

pathway A KEGGPathway-class object, usually as the result of the function parseKGML uniqueReaction

logical, to indicate whether several chemical reactions (identified by different KEGG reaction ID) should be treated as one (TRUE) or many (FALSE)

# Details

The direction of the graph is specified by the role of the compound in the reaction, the edges goes always out of 'substrate' and points to 'product'.

For now there is no wrapper to parse the KGML file directly into a reaction graph. In future there maybe one, but we don't want to confuse users with two similar functions to parse the file into a graph (since we assume that most users will need the protein graph, which can be conveniently parsed by parseKGML2Graph).

# Value

A directed graph with compounds as nodes and reactions as edges.

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

# References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

# See Also

KEGGPathway-class

### Examples

```
mapfile <- system.file("extdata/map00260.xml",package="KEGGgraph")
map <- parseKGML(mapfile)
cg <- KEGGpathway2reactionGraph(map, uniqueReaction=FALSE)
cg
nodes(cg)[1:3]
edges(cg)[1:3]</pre>
```

expandKEGGNode Expand KEGG node of paralogues

# Description

The function expands KEGG node of paralogues, and is mainly used internally. The end-users are not expected to call it unless they know exactly what they are doing.

### Usage

```
expandKEGGNode(node)
```

#### Arguments

node An object of KEGGNode-class

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

expandKEGGPathway Expand KEGG Pathway

### Description

The function expands paralogue nodes in KEGG pathway and returns expanded KEGG pathway, KEGG node and edge data is maintained.

### Usage

```
expandKEGGPathway(pathway)
```

# Arguments

pathway An object of KEGGPathway-class

### Details

The function expands nodes with paralogues in KEGG pathway and copy neccessary edges.

#### Value

An object of KEGGPathway-class

#### Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

#### See Also

expandKEGGNode

# Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
kegg.pathway <- parseKGML(sfile)
kegg.expandpathway <- expandKEGGPathway(kegg.pathway)</pre>
```

getDisplayName-methods

Get a character string as label for display

# Description

In KGML files, 'graph' element has a 'name' attribute to store the displaying name of a node, which is straighforward for end users. For example, biologists have no idea about a node 'hsa:1432' but its display name 'MAPK14' helps them to link this node to their knowledge. This method extract DisplayName from graph objects for KEGGNode and graph, where the method for graph returns the display names of its nodes.

#### Methods

```
object = "KEGGNode" An object of KEGGNode-class
object = "graph" A KEGG graph object
```

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

sapply(subnodes, getName)

### References

KGML Document Manual http://www.genome.jp/kegg/docs/xml/

#### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)
nodes <- nodes(pathway)
subnodes <- nodes[10:15]
sapply(subnodes, getDisplayName)
## compare them with getName, one 'displayName' may correspond to many paralogues</pre>
```

getEntryID-methods Get entry ID for single or list of KEGGNode or KEGGedge object(s)

#### Description

The method extracts EntryIDs from KEGGNode-class or KEGGEdge-class object(s).

In case of KEGGEdge-class objects, the entryID of the nodes involved in the binary are returned as a vector *in the order specified by the direction of the relation*, that is, if the edge is defined as A->B, then the entryID returned from the edge equals to c(getEntryID(A), getEntryID(B)).

# Methods

obj = "KEGGEdge" Object of KEGGEdge-class

obj = "list" A wrapper for list of KEGGNode-class or KEGGEdge-class objects

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

# References

KGML Document Manual http://www.genome.jp/kegg/docs/xml/

#### getKEGGID-methods

#### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)
nodes <- nodes(pathway)
node <- nodes[[7]]
getEntryID(node)
edges <- edges(pathway)
edge <- edges[[7]]
getEntryID(edge)
getEntryID(nodes[1:4])
getEntryID(edges[1:4])</pre>
```

getKEGGID-methods Get KEGG ID

# Description

Get KEGGID from a KEGGNode-class object.

The KEGGNode-class can be either another pathway (KEGGID in the form like 'hsa\d\*'), KEGG Gene ('hsa:\d\*') or compound ('cpd:C\d\*'). In case of the KEGG Gene ID, the organism prefix is removed when the value is returned.

#### Methods

object = "KEGGNode" An object of KEGGNode-class

# Examples

```
wntfile <- system.file("extdata/hsa04310.xml",package="KEGGgraph")
wnt <- parseKGML(wntfile)
nodes <- nodes(wnt)
getKEGGID(nodes[[1]])
getKEGGID(nodes[[26]])</pre>
```

getKEGGgeneLink-methods

Get KEGG gene link

# Description

Tranlsate a object into a link point to the gene on KEGG website. This method complies with the Gene link rule of the KEGG website.

# Methods

object = "character" A KEGGID, for example 'hsa:1423'

# Examples

getKEGGgeneLink("hsa:1423")

getKEGGnodeData

# Description

The 'get' methods extracts KEGG node (edge) attributes from a graph produced by calling parseKGML2Graph or KEGGpathway2Graph. The 'set' methods writes a list into the edge or node data.

# Usage

```
getKEGGnodeData(graph, n)
getKEGGedgeData(graph, n)
```

### Arguments

graph	a graph object by parsing KGML file, where KEGG node and edge attributes are maintained
n	optional character string, name of the desired node or edge. If is missing all node Data is returned

#### Details

Node and edge data is stored as list within environments in graphs to save memory and speed up graph manipulations. When using getKEGGnodeData or getKEGGedgeData is called, the list is extracted out of the environment and returned.

# Value

Either a list or single item of KEGGNode-class or KEGGEdge-class object(s).

#### Note

These functions will be unified into 'KEGGnodeData' and 'KEGGnodeData<-' forms.

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

#### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
gR <- parseKGML2Graph(sfile,expandGenes=TRUE)
getKEGGnodeData(gR,"hsa:4214")
getKEGGedgeData(gR,"hsa:4214~hsa:5605")</pre>
```

getKGMLurl

Get KGML file (url) with KEGG PATHWAY ID and (optional) organism

# Description

The function simply returns the KGML file url given KEGG PATHWAY ID. If the KEGG PATH-WAY ID contains no organism prefix, user can specify the 'organism' parameter. Otherwise the 'organism' option is ignored.

retrieveKGML is a simple wrapper to getKGMLurl, which downloads the KGML file with download.file in utils package.

kgmlNonmetabolicName2MetabolicName is used to translate non-metabolic pathway KGML URL to that of metabolic pathway. getCategoryIndepKGMLurl determines the correct URL to download by attempting both possibilities. They are mainly called internally.

# Usage

```
getKGMLurl(pathwayid, organism = "hsa")
retrieveKGML(pathwayid, organism, destfile,method="wget", ...)
kgmlNonmetabolicName2MetabolicName(destfile)
getCategoryIndepKGMLurl(pathwayid, organism="hsa", method="wget", ...)
```

# Arguments

pathwayid	KEGG PATHWAY ID, e.g. 'hsa00020'
organism	three-alphabet organism code, if pathwayid contains the ocde this option is ignored
destfile	Destination file, to which the remote KGML file should be saved
method	Method to be used for downloading files, passed to download.file function. Currently supports "internal", "wget" and "lynx"
	Parameters passed to download.file

### Details

The function getKGMLurl takes the pathway identifier (can be in the form of 'hsa00020' or with 'pathway' prefix, for example 'path:hsa00020'), and returns the url to download KGML file.

The mapping between pathway identifier and pathway name can be found by KEGGPATHNAME2ID (or reversed mappings) in KEGG.db package. See vignette for example.

retrieveKGML calls download. file to download the KGML file from KEGG FTP remotely.

# Value

KGML File URL of the given pathway.

So far the function does not check the correctness of the 'organism' prefix, it is the responsibility of the user to garantee the right spelling.

For Windows users, it is necessary to download and install wget program (http://gnuwin32. sourceforge.net/packages/wget.htm) to use the wget method to download files. Sometimes it may be necessary to modify searching path to add GnuWin32 folder (where wget execution file is located) and re-install R to make wget work.

Some user may face difficulty of retrieving KGML files when the download method is set to 'auto'. In this case setting the method to 'wget' may solve the problem (thanks to the report by Gilbert Feng).

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

#### Examples

```
getKGMLurl("hsa00020")
getKGMLurl("path:hsa00020")
getKGMLurl("00020",organism="hsa")
```

```
## NOT RUN
tmp <- tempfile()
retrieveKGML(pathwayid='00010', organism='cel', destfile=tmp, method="wget")</pre>
```

getName-methods Get 'name' attribute

# Description

Get 'name' attribute for given object, this method can be used for almost all objects implemented in KEGGgraph package to extract their name slot. See manual pages of individual objects for examples.

### Methods

object = "KEGGEdgeSubType" An object of KEGGEdgeSubType-class object = "KEGGNode" An object of KEGGNode-class object = "KEGGPathway" An object of KEGGPathway-class object = "KEGGPathwayInfo" An object of KEGGPathwayInfo-class object = "KEGGReaction" An object of KEGGReaction-class

#### Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

# References

KGML Document Manual http://www.genome.jp/kegg/docs/xml/

18

# Note

#### getNamedElement

### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)
## get pathway name
getName(pathway)
## get node name
nodes <- nodes(pathway)
getName(nodes[[2]])
## get edge name: it is not informative since the nodes are identified
## with file-dependent indices
edges <- edges(pathway)
getName(edges[[7]])
## get subtype name
subtype <- getSubtype(edges[[2]])[[1]]
getName(subtype)</pre>
```

getNamedElement Extract the value in a vector by name

# Description

The function extracts the value(s) in a named vector by given name(s), in case no element is found with the given name, NA will be returned

#### Usage

```
getNamedElement(vector, name)
```

#### Arguments

vector	A named vector of any data type
name	Wanted name

# Value

The elements with the given name, 'NA' in case no one was found

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

### Examples

```
vec <- c(first="Hamburg", second="Hoffenheim",third="Bremen")
getNamedElement(vec, "third")
getNamedElement(vec, "last")</pre>
```

getPathwayInfo-methods

Get KEGG pathway info

#### Description

KEGG stores additional information of the pathways in their KGML files, which can be extracted by this function.

The method returns the attributes of the pathway including its full title, short name, organism, image file link (which can be downloaded from KEGG website) and web link.

### Methods

object = "KEGGPathway" An object of KEGGPathway-class

#### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)
getPathwayInfo(pathway)</pre>
```

getReactions-methods

Get KEGG reactions

### Description

In KGML, the pathway element specifies one graph object with the *entry* elements as its nodes and the *relation* and *reaction* elements as its edges. The *relation* elements are saved as *edges* in objects of KEGGPathway-class, and the *reactions* elements are saved as a slot of the object, which can be retrieved with the function getReactions.

Regulatory pathways are always viewed as protein networks, so there is no 'reaction' information saved in their KGML files. Metabolic pathways are viewed both as both protein networks and chemical networks, hence the KEGGPathway-class object may have reactions information.

#### Methods

```
object = "KEGGPathway" An object of KEGGPathway-class
```

### Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

### References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

# See Also

KEGGPathway-class

### getRgraphvizEdgeNames

# Examples

```
mapfile <- system.file("extdata/map00260.xml", package="KEGGgraph")
maptest <- parseKGML(mapfile)
mapReactions <- getReactions(maptest)
mapReactions[1:3]</pre>
```

getRgraphvizEdgeNames

Get Rgraphviz compatitable edge names

# Description

Get Rgraphviz compatitable edge names, where the out- and in-nodes sharing a edge are concatenated by "~".

# Usage

getRgraphvizEdgeNames(graph)

#### Arguments

graph A graph object

# Value

A list of names, the order is determined by the edge order.

### Author(s)

Jitao David Zhang maito: j.zhang@dkfz.de

### References

Rgraphviz package

# Examples

```
tnodes <- c("Hamburg","Dortmund","Bremen", "Paris")
tedges <- list("Hamburg"=c("Dortmund", "Bremen"),
"Dortmund"=c("Hamburg"), "Bremen"=c("Hamburg"), "Paris"=c())
tgraph <- new("graphNEL", nodes = tnodes, edgeL = tedges)
getRgraphvizEdgeNames(tgraph)</pre>
```

getSubtype-methods Get subtype

#### Description

KEGG stores sub-type of interactions between entities in the KGML files, which can be extracted with this method. The descriptions for the subtypes can be explored at the KGML document manual in the references.

See KEGGEdge-class for examples. The method for graphs is a wrapper to extract all subtype information from one graph.

### Methods

**object = "graph"** A graph object of KEGGgraph. The method returns a list of subtypes in the same order of edges

object = "KEGGEdge" An object of KEGGEdge, which stores the subtype information

#### Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

#### References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)</pre>
```

```
edges <- edges(pathway)
subtype <- getSubtype(edges[[1]])
subtype</pre>
```

getTitle-methods Get title for given element

# Description

```
The methods get title attribute for given KGML element, for example for objects of KEGGPathway-
class or KEGGPathwayInfo-class
```

# Methods

```
object = "KEGGPathway" An object of KEGGPathway-class
object = "KEGGPathwayInfo" An object of KEGGPathwayInfo-class
```

#### getType-methods

#### Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

#### References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
pathway <- parseKGML(sfile)
getTitle(pathway)
pi <- getPathwayInfo(pathway)
getTitle(pi)</pre>
```

getType-methods Get type attribute

# Description

This method can be used to extract generic type attribute from several objects implemented in KEGGgraph package.

The meanings and descriptions of the types can be found at KGML manual listed in the reference.

### Methods

object = "KEGGEdge" An object of KEGGEdge-class
object = "KEGGNode" An object of KEGGNode-class
object = "KEGGReaction" An object of KEGGReaction-class

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

### References

KGML Manual http://www.genome.jp/kegg/docs/xml/

# Examples

```
mapfile <- system.file("extdata/map00260.xml", package="KEGGgraph")
maptest <- parseKGML(mapfile)
## node type
node <- nodes(maptest)[[3]]
getType(node)
## edge type
edge <- edges(maptest)[[5]]
getType(edge)</pre>
```

```
## reaction type
reaction <- getReactions(maptest)[[5]]
getType(reaction)</pre>
```

getValue-methods Get 'value' attribute

# Description

Get 'value' attribute, mainly used internally and is not expected to be called by users.

#### Methods

object = "KEGGEdgeSubType" An object of KEGGEdgeSubType-class

graphDensity Graph density

### Description

The graph density is defined as  $d = E/(V^*(V-1)/2)$  where E is the number of edges and V of nodes.

#### Usage

```
graphDensity(graph)
```

# Arguments

graph A graph object

# Details

The density of a graph lies between [0,1]

# Value

A value between [0,1]

### Author(s)

Jitao David Zhang j.zhang@dkfz.de

#### References

Aittokallio and Schwikowski (2006), Graph-based methods for analysing networks in cell biology, Briefings in Bioinformatics, 7, 243-255.

### isHomoList

### Examples

```
tnodes <- c("Hamburg","Dortmund","Bremen", "Paris")
tedges <- list("Hamburg"=c("Dortmund", "Bremen"),
"Dortmund"=c("Hamburg"), "Bremen"=c("Hamburg"), "Paris"=c())
tgraph <- new("graphNEL", nodes = tnodes, edgeL = tedges)
graphDensity(tgraph)</pre>
```

isHomoList

Determines whether a list is homogenous

# Description

If a list contains objects of the same class with the given class name, we call it a homogenous list and the function returns TRUE, otherwise it returns FALSE.

### Usage

```
isHomoList(list, class)
```

# Arguments

list	A list
class	The class name to be validated

#### Value

logical

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

# Examples

```
testlist <- list("home1"="Hamburg","home2"="Heidelberg",
"home3"="Tianjin")
isHomoList(testlist,"character")
testlist$lucky <- 16
isHomoList(testlist,"character")</pre>
```

```
kgmlFileName2PathwayName
```

Convert KGML file name to pathway name

# Description

The function uses KEGG package and converts KGML file name into human readable pathway name.

### Usage

```
kgmlFileName2PathwayName(filename)
```

#### Arguments

filename A KGML file name

# Details

So far it only supports KGML files organized by species.

NOTE: there is issue of package loading sequence to use this function: the 'KEGG.db' must be loaded before 'KEGGgraph' to use it properly. Otherwise the mget returns error of 'KEGG-PATHID2NAME' is not a environment. So far I don't where does this bug come from, so I commented out the examples.

#### Value

A character string of pathway name

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

mergeGraphs A function to merge KEGG graphs

#### Description

The function merges a list of KEGG graphs into one graph object. The merged graph have unique nodes, and edges are merged into non-duplicate sets.

For the reason of speed, mergeGraphs discards KEGG node and edge informations. To maintain them while merging graphs, please use mergeKEGGgraphs.

# Usage

mergeGraphs(list, edgemode = "directed")

# Arguments

list	A list of graph objects, which can be created by parseKGML2Graph
edgemode	Edge mode of the graph product, by default 'directed'

#### Details

The function takes a list of graphs and merges them into a new graph. The nodes of individual graphs must be unique. The function takes care of the removal of duplicated edges.

# Value

A directed graph

#### Note

It is known that graphs from C.elegance pathways have problem when merging, because the nodes name are not consistent betweeen edge records and entry IDs.

# Author(s)

Jitao David Zhang <j.zhang@dkfz.de>

#### See Also

parseKGML2Graph

mergeKEGGgraphs	Merge KEGG graphs, also merging KEGGNode and KEGGEdge at-
	tributes

### Description

mergeKEGGgraphs extends function mergeGraphs and merges a list of KEGG graphs. Both mergeGraphs and mergeKEGGgraphs can be used to merge graphs, while the latter form is able to merge the nodes and edges attributes from KEGG, so that the nodes and edges have a one-to-one mapping to the results from getKEGGnodeData and getKEGGEdgeData.

See details below.

# Usage

mergeKEGGgraphs(list, edgemode = "directed")

### Arguments

list	A list of named KEGG graphs
edgemode	character, 'directed' by default

### Details

mergeGraphs discards the node or edge attributes, hence getKEGGnodeData or getKEGGedgeData will return NULL on the resulting graph.

mergeKEGGgraphs calls mergeGraphs first to merge the graphs, then it also merges the KEG-GnodeData and KEGGedgeData.so that they are one-to-one mapped to the nodes and edges in the merged graph.

# Value

A graph with nodeData and edgeData

#### Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

# See Also

mergeGraphs

#### Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
gR <- parseKGML2Graph(sfile,expandGenes=TRUE)</pre>
```

wntfile <- system.file("extdata/hsa04310.xml",package="KEGGgraph")
wntR <- parseKGML2Graph(wntfile, expandGenes=TRUE)</pre>

graphlist <- list(mapkG=gR, wntG=wntR)
mergedKEGG <- mergeKEGGgraphs(graphlist)</pre>

mergedKEGG

neighborhood Return the neighborhood set of given vertices

### Description

The function returns the neighborhood set of given vertices in the form of list. Optionally user can choose to include the given vertices in the list, too.

#### Usage

neighborhood(graph, index, return.self = FALSE)

#### Arguments

graph	An object of graphNEL
index	Names of nodes, whose neighborhood set should be returned
return.self	logical, should the vertex itself also be returned?

#### parseEntry

#### Details

Let v be a vertex in a (di)graph, the out-neighborhood or successor set  $(N+(v), x \text{ belongs to } V(G) \text{ and } v \rightarrow x)$  and the in-neighborhood or predecessor set  $(N-(v), x \text{ belongs to } V(G) \text{ and } x \rightarrow v)$  are jointly returned.

The returned list is indexed by the given node indices, NULL is returned in case of non-existing node.

The nodes are unique, that is, duplicated nodes are removed in results.

### Value

A list indexed by the given node indices, each entry containing the neighborhood set of that node (or furthermore including that node).

### Author(s)

Jitao David Zhang <j.zhang@dkfz.de>

### References

D.B. West. Introduction to Graph Theory, Second Edition. Prentice Hall, 2001

### Examples

```
V <- c("Hamburg", "Stuttgart", "Berlin", "Paris", "Bremen")</pre>
E <- list("Hamburg"=c("Berlin", "Bremen"),</pre>
          "Stuttgart"=c("Berlin", "Paris"),
          "Berlin"=c("Stuttgart", "Bremen"),
          "Paris"=c("Stuttgart"),
          "Bremen"=c("Hamburg", "Berlin"))
g <- new("graphNEL", nodes=V, edgeL=E, edgemode="directed")</pre>
if(require(Rgraphviz) & interactive()) {
 plot(g, "neato")
}
## simple uses
neighborhood(g, "Hamburg")
neighborhood(g, c("Hamburg", "Berlin", "Paris"))
## in case of non-existing nodes
neighborhood(g, c("Stuttgart", "Ulm"))
## also applicable to non-directed graphs
neighborhood(ugraph(g), c("Stuttgart", "Berlin"))
```

parseEntry

Parse ENTRY elements of KGML document

#### Description

ENTRY elements contain information of nodes (proteins, enzymes, compounds, maps, etc) in KEGG pathways. 'parseEntry' function parses the elements into link {KEGGNode-class} or KEGGGroup-class objects. It is not expected to be called directly by the user.

#### Usage

parseEntry(entry)

### Arguments

entry XML node of KGML file

# Details

See http://www.genome.jp/kegg/docs/xml/ for more details about 'entry' as well as other elements in KGML files.

# Value

An object of link {KEGGNode} or (in case of a group node) link {KEGGGroup}

#### Author(s)

Jitao David Zhang <j.zhang@dkfz.de>

### References

http://www.genome.jp/kegg/docs/xml/

### See Also

parseGraphics, parseKGML, KEGGNode-class, KEGGGroup-class

parseGraphics Parse 'graphics' elements in KGML files

### Description

The function parses 'graphics' elements in KGML files, and it is mainly used internally.

# Usage

```
parseGraphics (graphics)
```

# Arguments

graphics XML node

# Details

The function is called by other parsing functions and not intended to be called directly by user.

### Value

An object of KEGGGraphics-class.

#### parseKGML

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

### References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

# See Also

KEGGGraphics-class

parseKGML	KGML file parser	

# Description

The function parses KGML files according to the KGML XML documentation.

# Usage

parseKGML(file)

# Arguments

file Name of KGML file

# Details

The function parses KGML file (depending on XML package).

# Value

An object of KEGGPathway-class.

### Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

# References

KGML Manual http://www.genome.jp/kegg/docs/xml/

# See Also

parseEntry, parseRelation, parseReaction, KEGGPathway-class,

# Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
kegg.pathway <- parseKGML(sfile)
kegg.pathway</pre>
```

parseKGML2Graph Parse KGML files into KEGG graph

# Description

This function is a wrapper for parseKGML and KEGGpathway2Graph. It takes two actions: first it reads in the KGML file and parses it into an object of KEGGPathway-class, the second step it calls KEGGpathway2Graph function to return the graph model.

### Usage

```
parseKGML2Graph(file, ...)
```

#### Arguments

file	Name of KGML file
	$other \ parameters \ passed \ to \ KEGG pathway 2 Graph, see \ KEGG pathway 2 Graph$

# Value

A graph object.

### Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

# Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
gR <- parseKGML2Graph(sfile,expandGenes=TRUE)
gR</pre>
```

parseKGMLexpandMaps

A convenient function to parse KGML and expand its containing maps into

### Description

The function does several tasks implemented in the KEGGgraph package in sequence to make expanding maps easier.

# Usage

```
parseKGMLexpandMaps(file, downloadmethod = "wget", genesOnly = TRUE, localdir,..
```

#### parsePathwayInfo

#### Arguments

<pre>downloadmethod     passed to download.file function as 'method', see its documentation :     more details</pre>	
more details	for
genesOnly logical, should only the genes nodes remain in the returned graph object?	
localdir character string, if specified, the function tries to read files with the same baname from a local directory, useful when there are file copies on the client.	ise
Other parameters passed to download.file	

### Details

In KEGG pathways there're usually pathways contained('cross-linked') in other pathways, for example see http://www.genome.jp/kegg/pathway/hsa/hsa04115.html, where p53 signalling pathway contains other two pathways 'apoptosis' and 'cell cycle'. This function parses these pathways (refered as 'maps' in KGML manual), download their KGML files from KEGG FTP website, parse them individually, and merge all the children pathway graphs with the parental pathway into one graph object. The graph is returned as the function value.

Since different graphs does not have unique node identifiers unless the genes are expanded, so by using this function user has to expand the genes. Another disadvantage is that so far due to the implementation, the KEGGnodeData and KEGGedgeData is lost during the merging. This however will probably be changed in the future version.

# Value

A directed graph object

# Author(s)

Jitao David Zhang j.zhang@dkfz.de

### References

KGML Document manual http://www.genome.jp/kegg/docs/xml/

#### See Also

for most users it is enough to use parseKGML2Graph

parsePathwayInfo Parse information of the pathway from KGML files

#### Description

The function parses the information of the given pathway from KGML files into an object of KEGGPathwayInfo-class. It is used internally and is not expected to be called by users directly.

# Usage

```
parsePathwayInfo(root)
```

#### parseReaction

# Arguments

root Root element of the KGML file

# Value

An object of KEGGPathwayInfo-class

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

# References

KGML Document Manual http://www.genome.jp/kegg/docs/xml/

parseReaction Parse reaction from KGML files

### Description

The function parses 'reaction' element in KGML files. It is used interally and not expected to be called by users.

# Usage

```
parseReaction (reaction)
```

# Arguments

reaction A node of the type 'reaction' in KGML files

# Details

See the reference manual for more information about 'reaction' type

# Value

```
An object of KEGGReaction-class
```

# Author(s)

Jitao David Zhang mail:j.zhang@dkfz.de

# References

KGML Document Manual http://www.genome.jp/kegg/docs/xml/

parseRelation Parse RELATION elements from KGML files

#### Description

RELATION elements in KGML files record the binary relationships between ENTRY elements, corresponding to (directed) edges in a graph. 'parseRelation' function parses RELATION elements into KEGGEdge-class objects from KGML files. It is not expected to be called directly by the user.

### Usage

```
parseRelation(relation)
```

# Arguments

relation XML node of KGML file

# Details

See http://www.genome.jp/kegg/docs/xml/ for more details about 'relation' as well as other elements in KGML files.

# Value

An object of link {KEGGEdge}.

# Author(s)

Jitao David Zhang <j.zhang@dkfz.de>

#### References

http://www.genome.jp/kegg/docs/xml/

# See Also

KEGGEdge-class, parseEntry

parseSubType Parse KGML relation subtype

#### Description

The function parses KGML relation subtype, called internally and not intended to be used by end users.

# Usage

```
parseSubType(subtype)
```

# Arguments

subtype KGML subtype node

# Value

An object of KEGGEdgeSubType-class

# Author(s)

Jitao David Zhang mailto: j.zhang@dkfz.de

plotKEGGgraph *Plot KEGG graph with Rgraphviz* 

# Description

The function provides a simple interface to Rgraphviz to render KEGG graph with custom styles. KEGGgraphLegend gives the legend of KEGG graphs

### Usage

```
plotKEGGgraph(graph, y = "neato", shortLabel = TRUE,
useDisplayName=TRUE, nodeRenderInfos, ...)
KEGGgraphLegend()
```

# Arguments

graph	A KEGG graph, by calling parseKGML2Graph
У	the layout method, neato by default
shortLabel	logical, should be short label used instead of full node name?
useDisplayName	
	logical, should the labels of nodes rendered as the 'display name' specified in the KGML file or render them simply with the node names?
nodeRenderInfos	
	List of node rendering info
	Other functions passed to renderGraph, not implemented for now

# Details

Users are not restricted to this function, alternatively you can choose other rendering functions.

# Value

The graph after layout and rendering is returned.

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

#### pvalue2asterisk

## Examples

```
opar <- par(ask=TRUE)
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
gR <- parseKGML2Graph(sfile,expandGenes=TRUE)
subs <- c("hsa:1432",edges(gR)$`hsa:1432`,"hsa:5778","hsa:5801","hsa:84867","hsa:11072",
gR.sub <- subGraph(subs, gR)
if(require(Rgraphviz))
plotKEGGgraph(gR.sub)
KEGGgraphLegend()
par(opar)</pre>
```

pvalue2asterisk Return common significance sign (asterisk) associated with given p

# Description

A p-value of 0.05, 0.01, 0.001 correspond to one, two or three asterisks. If 'sig.1' is set to TRUE, then the p-value of 0.1 returns '.'.

# Usage

```
pvalue2asterisk(pvalues, sig.1 = FALSE)
```

## Arguments

pvalues	A numeric value
sig.1	logical, whether the significance sign of 0.1 should be returned

# Value

A character string containing the signs

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

```
pvalue2asterisk(0.03)
pvalue2asterisk(0.007)
pvalue2asterisk(3e-5)
pvalue2asterisk(0.55)
```

queryKEGGsubgraph Query the subgraph of a given KEGG graph with Entrez GeneID (s)

## Description

Given a list of genes (identified by Entrez GeneID), the function subsets the given KEGG gragh of the genes as nodes (and maintaining all the edges between).

# Usage

```
queryKEGGsubgraph (geneids, graph, organism = "hsa", addmissing = FALSE)
```

#### Arguments

geneids	A vector of Entrez GeneIDs
graph	A KEGG graph
organism	a three-alphabet code of organism
addmissing	logical, in case the given gene is not found in the graph, should it be added as single node to the subgraph?

#### Details

This function solves the questions like 'How is the list of gene interact with each other in the context of pathways?'

Limited by the translateKEGGID2GeneID, this function supports only human for now. We are working to include other organisms.

If 'addmissing' is set to TRUE, the missing gene in the given list will be added to the returned subgraph as single nodes.

## Value

A subgraph with nodes representing genes and edges representing interactions.

# Author(s)

Jitao David Zhang <j.zhang@dkfz.de>

#### See Also

translateGeneID2KEGGID

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
gR <- parseKGML2Graph(sfile,expandGenes=TRUE)
geneids <- c(5594, 5595, 6197, 5603, 1843,5530, 5603)
sub <- queryKEGGsubgraph(geneids, gR)
if(require(Rgraphviz) && interactive()) {
   plot(sub, "neato")
}</pre>
```

### randomSubGraph

```
## add missing nodes
list2 <- c(geneids, 81029)
sub2 <- queryKEGGsubgraph(list2, gR,addmissing=TRUE)
if(require(Rgraphviz) && interactive()) {
   plot(sub2, "neato")
}</pre>
```

randomSubGraph Randomly subset the given graph

## Description

The function is intended to be a test tool. It subset the given graph repeatedly.

## Usage

```
randomSubGraph(graph, per = 0.25, N = 10)
```

# Arguments

graph	A graph object
per	numeric, the percentage of the nodes to be sampled, value between $(0,1)$
Ν	Repeat times

## Value

The function is called for its side effect, NULL is returned

# Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

```
tnodes <- c("Hamburg","Dortmund","Bremen", "Paris")
tedges <- list("Hamburg"=c("Dortmund", "Bremen"),
"Dortmund"=c("Hamburg"), "Bremen"=c("Hamburg"), "Paris"=c())
tgraph <- new("graphNEL", nodes = tnodes, edgeL = tedges)
randomSubGraph(tgraph, 0.5, 10)</pre>
```

splitKEGGgroup Split KEGG group

#### Description

The function split 'group' entries in KGML files. Most of the cases they are complexes. During the splitting the function copies the edges between groups and nodes (or between groups and groups) correspondingly, so that the existing edges also exist after the groups are split.

# Usage

```
splitKEGGgroup(pathway)
```

## Arguments

pathway An object of KEGGPathway-class

# Details

By default the groups (complexes) in KEGG pathways are split.

# Value

An object of KEGGPathway-class

## Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

## References

KGML Manual http://www.genome.jp/kegg/docs/xml/

## See Also

KEGGpathway2Graph

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
kegg.pathway <- parseKGML(sfile)
kegg.pathway.split <- splitKEGGgroup(kegg.pathway)
## compare the different number of edges
length(edges(kegg.pathway))</pre>
```

subGraphByNodeType Subset KEGG graph by node types

## Description

The function subsets KEGG graph by node types, mostly used in extracting gene networks.

## Usage

```
subGraphByNodeType(graph, type = "gene", kegg=TRUE)
```

## Arguments

graph	A KEGG graph object produced by calling parseKGML2Graph
type	node type, see KEGGNodeType for details
kegg	logical, should the KEGG Node and Edge attributes be maintained during the subsetting? By default set to 'TRUE'

## Value

A subgraph of the original graph

## Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

## Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
sGraph <- parseKGML2Graph(sfile,expandGenes=TRUE, genesOnly=FALSE)
sGraphGene <- subGraphByNodeType(sGraph, type="gene")</pre>
```

subKEGGgraph Subset KEGG graph, including subsetting node and edge attributes

# Description

subKEGGgraph extends generic method subGraph and subsets the KEGG graph. Both 'sub-KEGGgraph' and 'subGraph' can be used to subset the graph, the difference lies in whether the node and edge attributes from KEGG are also subset (subKEGGgraph) or not (subGraph).

See details below.

# Usage

```
subKEGGgraph(nodes, graph)
```

#### Arguments

nodes	Node names to subset
graph	A graph parsed from KGML files, produced by parseKGML2Graph, KEGGpathway2Graph
	or parseKGMLexpandMaps

## Details

subGraph does not subset the node or edge attributes, hence the results of getKEGGnodeData and getKEGGedgeData does not map to the nodes and edges in the subgraph in a one-to-one manner, with attributes of removed nodes and edges still remaining in the subGraph.

subKEGGgraph calls subGraph first to subset the graph, and then it also subsets the KEGGnodeData and KEGGedgeData so that they are one-to-one mapped to the nodes and edges in the subgraph.

# Value

A graph with nodeData and edgeData.

## Author(s)

Jitao David Zhang mailto:j.zhang@dkfz.de

## Examples

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
gR <- parseKGML2Graph(sfile,expandGenes=TRUE)
subs <- c("hsa:1432",edges(gR)$`hsa:1432`,"hsa:5778","hsa:5801",
"hsa:84867","hsa:11072","hsa:5606","hsa:5608","hsa:5494","hsa:5609")
gR.keggsub <- subKEGGgraph(subs, gR)
gR
gR.keggsub</pre>
```

subtypeDisplay-methods

Get display information for relation subtypes

# Description

To render KEGG pathway graphs, we have created a custom style of edges to represent their subtypes. 'subtypeDisplay' extracts this information

# Methods

```
object = "graph" An KEGG graph
object = "KEGGEdge" An object of KEGGEdge-class
object = "KEGGEdgeSubType" An object of KEGGEdgeSubType-class
```

#### Description

Colorectal cancer dataset provided by SPIA package. It is just a copy during the development of SPIA package in case the package is not available. It will be removed when the SPIA package is stable.

see the description of SPIA package.

## Usage

data(colorectalcancerSPIA)

#### Format

see the format of SPIA package.

## Source

Yi Hong and Kok Sun Ho and Kong Weng Eu and Peh Yean Cheah, A susceptibility gene set for early onset colorectal cancer that integrates diverse signaling pathways: implication for tumorigenesis, Clin Cancer Res, 2007, 13(4),1107-14.

```
translateKEGGID2GeneID
```

Translate between KEGGID and Entrez Gene ID

## Description

translateKEGGID2GeneID translates KEGGID to NCBI Entrez Gene ID, and translateGeneID2KEGGID translates Entrez Gene ID back to KEGGID.

# Usage

```
translateKEGGID2GeneID(x, organism="hsa")
translateGeneID2KEGGID(x, organism="hsa")
```

#### Arguments

Х	KEGGID, e.g. 'hsa:1432', or Entrez Gene ID, e.g. '1432'
organism	Three alphabet code for organisms. The mapping between the orgniams and
	<pre>codes can be found at http://www.genome.jp/kegg/kegg3.html</pre>

#### top

#### Details

The KEGGID are unique identifiers used by KEGG PATHWAY to identify gene products. After parsing the KEGG pathway into graph, the graph use KEGGID as its nodes' names.

translateKEGGID2GeneID converts KEGGIDs into entrez GeneID, which can be translated to other types of identifiers, for example with biomaRt package or organism-specific annotation packages. See vignette for examples.

translateKEGG2GeneID is maintained for back-compatibility and wrapps translateKEGGID2GeneID.

#### Value

Entrez GeneID of the given KEGG ID(s)

#### Note

This function works so far only with human KEGGIDs, since for them the Entrez GeneID can be derived easily with removing the organism prefix.

The complete functional function will be implemented in the later release of the package.

## Author(s)

Jitao David Zhang

#### Examples

```
egNodes <- c("hsa:1432", "hsa:11072")
translateKEGGID2GeneID(egNodes)
translateGeneID2KEGGID("1432")</pre>
```

translateKEGGgraph Tranlate the KEGG graph from being indexed by KEGGID to another

#### Description

The function translates the KEGG graph into a graph of equivalant topology while index with unique identifiers given by user. The new identifiers could be, for example, GeneSymbol or other identifiers mapped to KEGGID.

# Usage

```
translateKEGGgraph(graph, newNodes)
```

#### Arguments

graph	A KEGG graph
newNodes	A character vector giving the new nodes, must be of the same length and same order of the nodes of the given graph

# Details

The function is still experimental and users are welcomed to report any difficulties

# Value

Another graph indexed by the given identifier

# Author(s)

Jitao David Zhang <j.zhang@dkfz.de>

```
sfile <- system.file("extdata/hsa04010.xml",package="KEGGgraph")
gR <- parseKGML2Graph(sfile,expandGenes=TRUE)
subG <- subKEGGgraph(c("hsa:1848","hsa:1432","hsa:2002","hsa:8986"),gR)
symbols <- c("DUSP6","MAPK14","ELK1","RPS6KA4")
sub2G <- translateKEGGgraph(subG, symbols)
sub2G
nodes(sub2G)
if(require(Rgraphviz) & interactive()) {
plot(sub2G, "neato")
}</pre>
```

# Index

\*Topic IO getKGMLurl, 17 parseEntry, 29 parsePathwayInfo, 33 parseReaction, 34 parseRelation, 35 \*Topic classes KEGGEdge-class, 1 KEGGEdgeSubType-class, 2 KEGGGraphics-class,4 KEGGGroup-class, 5 KEGGNode-class, 6 KEGGPathway-class, 7 KEGGPathwayInfo-class, 8 KEGGReaction-class,9 \*Topic datasets KEGGEdgeSubtype, 3 top, 43 \*Topic **methods** getDisplayName-methods, 13 getEntryID-methods, 14 getKEGGgeneLink-methods, 15 getKEGGID-methods, 15 getName-methods, 18 getPathwayInfo-methods, 20 getReactions-methods, 20 getSubtype-methods, 22 getTitle-methods, 22 getType-methods, 23 getValue-methods, 24 subtypeDisplay-methods, 42 download.file,33 edges, KEGGPathway, ANY-method

(KEGGPathway-class), 7

(KEGGPathway-class),7

(KEGGPathway-class),7

edges, KEGGPathway-method

edges<-(KEGGPathway-class),7

edges<-, KEGGPathway-method

entryID<-(KEGGNode-class), 6

(KEGGEdge-class), 1

entryID<-, KEGGEdge-method

```
entryID<-, KEGGNode-method
       (KEGGNode-class), 6
expandKEGGNode, 12, 13
expandKEGGPathway, 13
getCategoryIndepKGMLurl
       (getKGMLurl), 17
getComponent (KEGGGroup-class), 5
getComponent, KEGGGroup-method
       (KEGGGroup-class), 5
getComponent, KEGGNode-method
       (KEGGNode-class), 6
getDisplayName
       (getDisplayName-methods),
       13
getDisplayName,graph-method
       (getDisplayName-methods),
       13
getDisplayName, KEGGNode-method
       (getDisplayName-methods),
       13
getDisplayName-methods, 13
getEntryID (getEntryID-methods),
       14
getEntryID, KEGGEdge-method
       (getEntrvID-methods), 14
getEntryID, KEGGNode-method
       (getEntryID-methods), 14
getEntryID, list-method
       (getEntryID-methods), 14
getEntryID-methods, 14
getKEGGedgeData, 10, 28, 42
getKEGGedgeData
       (getKEGGnodeData), 16
getKEGGgeneLink
       (getKEGGgeneLink-methods),
       15
getKEGGgeneLink, character-method
       (getKEGGgeneLink-methods),
       15
getKEGGgeneLink-methods, 15
getKEGGID (getKEGGID-methods), 15
getKEGGID, KEGGNode-method
       (getKEGGID-methods), 15
```

## INDEX

getKEGGID-methods, 15 getKEGGnodeData, 10, 16, 28, 42 getKGMLurl, 17 getName (getName-methods), 18 getName, KEGGEdge-method (KEGGEdge-class), 1 getName, KEGGEdgeSubType-method (KEGGEdgeSubType-class), 2 getName, KEGGEdgeSubtype-method (getName-methods), 18 getName, KEGGNode-method (getName-methods), 18 getName, KEGGPathway-method (KEGGPathway-class), 7 getName, KEGGPathwayInfo-method (getName-methods), 18 getName, KEGGReaction-method (KEGGReaction-class), 9 getName-methods, 18 getNamedElement, 19 getPathwayInfo (getPathwayInfo-methods), 20 getPathwayInfo, KEGGPathway-method (getPathwayInfo-methods), 20 getPathwayInfo-methods, 20 getProduct (KEGGReaction-class), 9 getProduct, KEGGReaction-method (KEGGReaction-class), 9 getReactions (getReactions-methods), 20 getReactions, KEGGPathway-method (getReactions-methods), 20 getReactions-methods, 20 getRgraphvizEdgeNames, 21 getSubstrate (KEGGReaction-class), 9 getSubstrate, KEGGReaction-method (KEGGReaction-class), 9 getSubtype (getSubtype-methods), 22 getSubtype, graph-method (getSubtype-methods), 22 getSubtype, KEGGEdge-method (getSubtype-methods), 22 getSubtype-methods, 22 getTitle(getTitle-methods), 22 getTitle, KEGGPathway-method (KEGGPathway-class), 7 getTitle, KEGGPathwayInfo-method (KEGGPathwayInfo-class), 8

getTitle-methods, 22 getType (getType-methods), 23 getType, KEGGEdge-method (getType-methods), 23 getType, KEGGNode-method (getType-methods), 23 getType, KEGGReaction-method (getType-methods), 23 getType-methods, 1 getType-methods, 23 getValue (getValue-methods), 24 getValue, KEGGEdgeSubType-method (KEGGEdgeSubType-class), 2 getValue,KEGGEdgeSubtype-method (getValue-methods), 24 getValue-methods, 24 graphDensity, 24

# isHomoList, 25

KEGGEdge-class, 3, 6-8, 14, 16, 22, 23, 35,42 KEGGEdge-class, 1 KEGGEdgeSubType, 1 KEGGEdgeSubtype, 3 KEGGEdgeSubType-class, 18, 24, 36, 42 KEGGEdgeSubType-class, 2 KEGGEdgeType (KEGGEdgeSubtype), 3 KEGGGraphics, 6KEGGGraphics-class, 30, 31 KEGGGraphics-class, 4 KEGGgraphLegend (plotKEGGgraph), 36 KEGGGroup-class, 6, 29, 30 KEGGGroup-class, 5 KEGGNode, 5 KEGGNode-class, 2, 5, 7, 8, 12, 14-16, 18, 23.30 KEGGNode-class, 6 KEGGNodeType, 41 KEGGNodeType (KEGGEdgeSubtype), 3 KEGGPathway-class, 10-13, 18, 20, 22, 31, 32, 40 KEGGPathway-class,7 KEGGpathway2Graph, 6, 10, 16, 32, 40, 42 KEGGpathway2reactionGraph, 11 KEGGPathwayInfo-class, 7, 18, 22, 33, 34 KEGGPathwayInfo-class, 8 KEGGReaction-class, 7, 8, 18, 23, 34 KEGGReaction-class,9 kgmlFileName2PathwayName, 26

## INDEX

```
kgmlNonmetabolicName2MetabolicName (getKGMLurl), 17
```

mergeGraphs, 26, 28 mergeKEGGgraphs, 26, 27

name<-(KEGGNode-class),6
name<-,KEGGNode-method
 (KEGGNode-class),6
neighborhood,28
nodes,KEGGPathway-method
 (KEGGPathway-class),7
nodes<-,KEGGPathway,ANY-method
 (KEGGPathway-class),7</pre>

queryKEGGsubgraph, 38

randomSubGraph, 39
retrieveKGML(getKGMLurl), 17

```
setKEGGedgeData
       (getKEGGnodeData), 16
setKEGGnodeData
       (getKEGGnodeData), 16
show, KEGGEdge-method
       (KEGGEdge-class), 1
show, KEGGEdgeSubType-method
       (KEGGEdgeSubType-class), 2
show, KEGGNode-method
       (KEGGNode-class), 6
show, KEGGPathway-method
       (KEGGPathway-class),7
show, KEGGPathwayInfo-method
       (KEGGPathwayInfo-class), 8
show, KEGGReaction-method
       (KEGGReaction-class), 9
splitKEGGgroup, 40
subGraphByNodeType, 41
subKEGGgraph, 41
```

subtypeDisplay (subtypeDisplay-methods), 42 subtypeDisplay,graph-method (subtypeDisplay-methods), 42 subtypeDisplay, KEGGEdge-method (subtypeDisplay-methods), subtypeDisplay, KEGGEdgeSubType-method (subtypeDisplay-methods), 42 subtypeDisplay-methods, 42 top, 43 translateGeneID2KEGGID, 38 translateGeneID2KEGGID (translateKEGGID2GeneID), 43 translateKEGG2GeneID (translateKEGGID2GeneID), 43

translateKEGGgraph, 44 translateKEGGID2GeneID, 38, 43

48