# Package 'rBiopaxParser'

November 22, 2012

Type Package
Title Parses BioPax files and represents them in R
<b>Version</b> 0.99.5
Date 2012-11-22
Author Frank Kramer
Maintainer Frank Kramer <dev@frankkramer.de></dev@frankkramer.de>
<b>Description</b> Parses BioPAX files and represents them in R, at the moment BioPAX level 2 and level 3 are supported.
<b>License</b> GPL (>= 2)
Imports XML
Suggests Rgraphviz, RCurl, graph
URL https://github.com/frankkramer/rBiopaxParser
Collate 'biopax2Classes.R' 'downloadBiopaxData.R' 'helperFunctions.R' 'modifyBiopax.R' 'parseBiopax.R' 'rBiopaxParser package.R' 'selectBiopax.R' 'visualizeBiopax.R' 'writeBiopax.R'
R topics documented:
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rBiopaxParser-package Parses BioPax level files and represents them in R

# Description

Parses BioPax files and represents them in R

#### **Details**

rBiopaxParser is a...

Package: rBiopaxParser
Type: Package
Version: 0.15
Date: 2012-08-22
License: GPL (>= 2)

# Author(s)

Frank Kramer < dev@frankkramer.de>

# Examples

```
## Not run: biopax = readBiopax(file="biopaxmodel.owl")
```

addBiochemicalReaction

This function adds a new biochemical reaction to the biopax model.

### **Description**

This function adds a new biochemical reaction of class biochemicalReaction to the biopax model. This is a convenience function, internally the function addBiopaxInstance is called with properties LEFT and RIGHT set.

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# Usage

```
addBiochemicalReaction(biopax, LEFT = c(), RIGHT = c(),
  id = NULL)
```

#### **Arguments**

biopax	A biopax model
LEFT	vector of strings. IDs of the physicalEntityParticipant instances that are on the left side of this reaction.
RIGHT	vector of strings. IDs of the physicalEntityParticipant instances that are on the right side of this reaction.
id	string. ID for the control. If NULL a new ID is generated with prefix "biochemicalReaction".

#### Value

Returns the biopax model with the added pathway.

#### Author(s)

fkramer

# **Examples**

```
biopax = createBiopax(level=2)
biopax = addPhysicalEntity(biopax, class="protein", id="p_id1", NAME="protein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id1", id="PEP_p_id1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id2", NAME="protein2")
biopax = addPhysicalEntityParticipant(biopax, "p_id2", id="PEP_p_id2")
biopax = addBiochemicalReaction(biopax, LEFT=c("PEP_p_id1"), RIGHT=c("PEP_p_id2"), id="biochem_id_1")
biopax$df
```

addBiopaxInstance

This function adds a new instance to an existing biopax model.

#### **Description**

This function adds a new instance to an existing biopax model. "properties" is a named list of vectors, with the vector name as the name of the property and every entry of the vector a property value. Please note: case sensitivity! In Biopax Level 2 all properties are written in all capital letters. This will change in Biopax Level 3.

# Usage

```
addBiopaxInstance(biopax, class, id,
  properties = list(NAME = c()), verbose = TRUE)
```

addBiopaxInstances 5

#### **Arguments**

biopax A biopax model class string. Class name

id string. ID of the instanceproperties named list of properties.

verbose logical. Be verbose about what was added.

#### Value

Returns the supplied biopax model with the new instance added.

#### Author(s)

Frank Kramer

#### **Examples**

```
biopax = createBiopax(level=2)
biopax = addBiopaxInstance(biopax, class="protein", id="id1", properties=list(NAME="protein1",SYNONYMS="p1"))
biopax$df
```

addBiopaxInstances

This function adds new instances to an existing biopax model.

#### **Description**

This function adds new instances (supplied as a compatible data.frame) to an existing biopax model via rbind. Usually you want to start out at createBiopax and addPhysicalEntity and work your way up the ontology ladder.

### Usage

```
addBiopaxInstances(biopax, newInstancesDF)
```

#### **Arguments**

biopax A biopax model

newInstancesDF data.frame. Compatible with internal Biopax Level 2 implementation.

#### Value

Returns the supplied biopax model with the new instances added.

#### Author(s)

Frank Kramer

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#### **Examples**

```
# load data
data(biopax2example)
biopax_temp = createBiopax(level=2)
biopax_temp = addBiopaxInstance(biopax_temp, class="protein", id="id1", properties=list(NAME="protein1",SYNONYM
selectInstances(biopax_temp)
biopax = addBiopaxInstances(biopax, selectInstances(biopax_temp))
```

addControl

This function adds a new control to the biopax model.

# Description

This function adds a new interaction of class control to the biopax model. This is a convenience function to add controls, internally the function addBiopaxInstance is called with properties CONTROL-TYPE, CONTROLLER and CONTROLLED set.

### Usage

```
addControl(biopax,
  CONTROL_TYPE = c("ACTIVATION", "INHIBITION"),
  CONTROLLER = "", CONTROLLED = c(), id = NULL)
```

#### **Arguments**

biopax	A biopax model
CONTROL_TYPE	string. Specifies wether this is an activating or inhibiting control.
CONTROLLER	string. ID of the physicalEntityParticipant instance that is the controller of this interaction.
CONTROLLED	vector of strings. IDs of the interaction and/or pathway instances that are being controlled.
id	string. ID for the control. If NULL a new ID is generated with prefix "control".

# Value

Returns the biopax model with the added pathway.

### Author(s)

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#### **Examples**

```
biopax = createBiopax(level=2)
biopax = addPhysicalEntity(biopax, class="protein", id="p_id1", NAME="protein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id1", id="PEP_p_id1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id2", NAME="protein2")
biopax = addPhysicalEntityParticipant(biopax, "p_id2", id="PEP_p_id2")
biopax = addBiochemicalReaction(biopax, LEFT=c("PEP_p_id1"), RIGHT=c("PEP_p_id2"), id="biochem_id_1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id3", NAME="controllerProtein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id3", id="PEP_p_id3")
biopax = addControl(biopax, CONTROL_TYPE="ACTIVATION", CONTROLLER="PEP_p_id3", CONTROLLED="biochem_id_1", id="c_biopax$df
```

addhash

Adds a hash in front of a string

#### **Description**

Adds a hash in front of a string

#### Usage

addhash(x)

# Arguments

Х

A string to be preceded by a hash

#### Value

The supplied string with a hash "#" pasted in front of it.

#### Author(s)

Frank Kramer

addns

Add a namespace tag to the supplied classname string

# Description

This function takes the input classname, checks if it already has a namespace, and if not pastes the namespace tag with a dividing ":" in front of it.

#### Usage

```
addns(classname, namespace = "bp")
```

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#### **Arguments**

classname A string containing a classname namespace A string containing a namespace

#### Value

If the classname is not preceded by a namespace yet, the supplied namespace is pasted in front of it and returned.

#### Author(s)

Frank Kramer

addPathway This function adds a new pathway to the biopax model.

# Description

This function adds a new pathway + its PATHWAY-COMPONENTS (references to interaction/pathways/pathwaySteps)

### Usage

```
addPathway(biopax, NAME, PATHWAY_COMPONENTS = c(),
  id = NULL, ORGANISM = NULL, COMMENT = NULL)
```

# **Arguments**

biopax A biopax model

NAME string. Name of the pathway

PATHWAY\_COMPONENTS

character vector. IDs of the pathway components. This must be IDs of instances

of type interaction/pathway/pathwayStep (or their subclasses).

id string. ID for the pathway. If NULL a new ID is generated with prefix "path-

way".

ORGANISM string. Organism property of the pathway. optional.

COMMENT string. An optional comment

#### Value

Returns the biopax model with the added pathway.

# Author(s)

#### **Examples**

```
biopax = createBiopax(level=2)
biopax = addPhysicalEntity(biopax, class="protein", id="p_id1", NAME="protein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id1", id="PEP_p_id1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id2", NAME="protein2")
biopax = addPhysicalEntityParticipant(biopax, "p_id2", id="PEP_p_id2")
biopax = addBiochemicalReaction(biopax, LEFT=c("PEP_p_id1"), RIGHT=c("PEP_p_id2"), id="biochem_id_1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id3", NAME="controllerProtein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id3", id="PEP_p_id3")
biopax = addPostorol(biopax, CONTROL_TYPE="ACTIVATION", CONTROLLER="PEP_p_id3", CONTROLLED="biochem_id_1", id="c_biopax = addPathway(biopax, NAME="mypathway1", PATHWAY_COMPONENTS=c("c_id1"), id="pw_id1")
biopax$df
```

addPathwayComponents

This function adds pathway components to an existing pathway

#### **Description**

This function adds pathway components to an existing pathway. Property PATHWAY-COMPONENTS are references to IDs of interaction/pathways/pathwaySteps (or subclasses of those)

#### Usage

```
addPathwayComponents(biopax, id,
   PATHWAY_COMPONENTS = c())
```

#### **Arguments**

biopax A biopax model

id string. ID for the pathway

PATHWAY\_COMPONENTS

character vector. IDs of the pathway components. This must be IDs of instances of type interaction/pathway/pathwayStep (or their subclasses).

#### Value

Returns the biopax model with the pathway components added to the pathway

#### Author(s)

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#### **Examples**

```
biopax = createBiopax(level=2)
biopax = addPhysicalEntity(biopax, class="protein", id="p_id1", NAME="protein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id1", id="PEP_p_id1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id2", NAME="protein2")
biopax = addPhysicalEntityParticipant(biopax, "p_id2", id="PEP_p_id2")
biopax = addBiochemicalReaction(biopax, LEFT=c("PEP_p_id1"), RIGHT=c("PEP_p_id2"), id="biochem_id_1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id3", NAME="controllerProtein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id3", id="PEP_p_id3")
biopax = addControl(biopax, CONTROL_TYPE="ACTIVATION", CONTROLLER="PEP_p_id3", CONTROLLED="biochem_id_1", id="c_biopax = addPathway(biopax, NAME="mypathway1", PATHWAY_COMPONENTS=c(), id="pw_id1")
biopax = addPathwayComponents(biopax, id="pw_id1", PATHWAY_COMPONENTS=c("c_id1"))
biopax$df
```

addPhysicalEntity

This function adds a new physical entity.

#### **Description**

This function adds a new physical entity of chosen class to the biopax model. This is a convenience function to add physical entities, internally the function addBiopaxInstance is called with properties NAME and ORGANISM set.

# Usage

```
addPhysicalEntity(biopax,
  class = c("dna", "rna", "protein", "smallMolecule", "complex")[1],
  NAME, id = NULL, ORGANISM = NULL, COMMENT = NULL)
```

#### **Arguments**

biopax	A biopax model
class	string. Class of the physical entity to add, choose from c("dna", "rna", "protein", "smallMolecule", "complex
NAME	string. Name of the new physical entity
id	string. ID for the physical entity. If NULL a new ID is generated with prefix "physicalEntity".
ORGANISM	string. Organism property of the molecule. optional.
COMMENT	string. An optional comment

#### Value

Returns the biopax model with the added physical entity.

#### Author(s)

#### **Examples**

```
biopax = createBiopax(level=2)
biopax = addBiopaxInstance(biopax, class="protein", id="id1", properties=list(NAME="protein1", COMMENT="this is my
biopax$df
biopax = addPhysicalEntity(biopax, class="protein", id="id2", NAME="protein2", COMMENT="This is a protein added us
biopax$df
```

addPhysicalEntityParticipant

This function adds a new physical entity participant.

#### **Description**

This function adds a new physical entity participant instance, which is a placeholder for physicalEntity class instances in interactions. This is a convenience function to add physicalEntityParticipant instances, internally the function addBiopaxInstance is called.

### Usage

```
addPhysicalEntityParticipant(biopax,
  referencedPhysicalEntityID, id = NULL)
```

#### **Arguments**

biopax A biopax model referencedPhysicalEntityID

string. ID the new physicalEntity instance to reference here.

id string. ID for the physical entity participant. If NULL a new ID is generated

with prefix "physicalEntityParticipant".

#### Value

Returns the biopax model with the added physicalEntityParticipant.

# Author(s)

fkramer

#### **Examples**

```
biopax = createBiopax(level=2)
biopax = addPhysicalEntity(biopax, class="protein", id="p_id1", NAME="protein1")
biopax = addPhysicalEntityParticipant(biopax, "p_id1", id="PEP_p_id1")
biopax = addPhysicalEntity(biopax, class="protein", id="p_id2", NAME="protein2")
biopax = addPhysicalEntityParticipant(biopax, "p_id2", id="PEP_p_id2")
biopax = addBiochemicalReaction(biopax, LEFT=c("PEP_p_id1"), RIGHT=c("PEP_p_id2"), id="biochem_id1")
biopax$df
```

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 $add {\tt Properties To Biopax Instance}$ 

This function adds new properties to an existing biopax instance.

#### **Description**

This function adds new properties to an existing biopax instance.

# Usage

```
addPropertiesToBiopaxInstance(biopax, id, properties)
```

### **Arguments**

biopax A biopax model

id string. ID of the instanceproperties named list of properties.

#### Value

Returns the supplied biopax model with new properties added to this instance.

#### Author(s)

Frank Kramer

#### **Examples**

```
biopax = createBiopax(level=2)
biopax = addBiopaxInstance(biopax, class="protein", id="id1", properties=list(NAME="protein1",SYNONYMS="p1"))
biopax$df
biopax = addPropertiesToBiopaxInstance(biopax, id="id1", properties=list(COMMENT="this is my first protein!"))
biopax$df
```

biopax

Biopax example data set

### **Description**

A dataset containing two regulatory pathways encoded in Biopax Level 2 and parsed in via read-Biopax().

#### **Format**

An example biopax model parsed in via readBiopax.

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### **Examples**

```
data(biopax2example)
biopax
```

calcGraphOverlap

This function calculates the overlap of 2 graphs

### **Description**

This function calculates the overlap of supplied graph1 with graph2. Layout and weights of graph1 are kept.

# Usage

```
calcGraphOverlap(graph1, graph2)
```

### **Arguments**

graph1 graphNEL graph2 graphNEL

### Value

Returns a list containing the compared graphs and edge- and node-wise overlap between them.

### Author(s)

Frank Kramer

# **Examples**

```
# load data
data(biopax2example)
pwid1 = "pid_p_100002_wntpathway"
pwid2 = "pid_p_100146_hespathway"
mygraph1 = pathway2RegulatoryGraph(biopax, pwid1)
mygraph2 = pathway2RegulatoryGraph(biopax, pwid2)
calcGraphOverlap(mygraph1,mygraph2)
```

checkValidity

This function checks the supplied biopax model for validity.

# Description

This function checks the supplied biopax model for validity, concerning classes, properties, etc. Not yet implemented. Called internally by writeBiopax.

#### Usage

checkValidity(biopax)

### **Arguments**

biopax

A biopax model

#### Value

logical. Returns TRUE is the biopax model is valid Biopax Level 2, or FALSE otherwise.

### Author(s)

Frank Kramer

CLASS\_INHERITANCE

CLASS\_INHERITANCE

# **Description**

Class inheritance relationships in Biopax Level 2.

#### **Format**

A data frame with 46 rows and 2 columns

#### **Details**

A data.frame listing all direct superclasses for every Biopax Level 2 class. The variables are as follows:

- class. Name of the class
- superclass. Name of the superclass

CLASS\_PROPERTIES 15

# **Description**

Class properties in Biopax Level 2.

#### **Format**

A data frame with 106 rows and 4 columns

#### **Details**

A data.frame listing all direct properties for every Biopax Level 2 class. Together with CLASS\_INHERITANCE this allows to list all properties, including the inherited ones, of every class.

The variables are as follows:

- · class. Name of the class
- property. Name of the superclass
- property\_type.Type of the property, value or reference
- cardinality. Maximum allowed cardinality of a property. Many properties may only be singular.

colorGraphNodes	This function colors the nodes of a graph.

### **Description**

This function colors nodes of a graph, usually this is used to color subgraphs or add a color hue correlating with the expression level or fold change to the molecules.

# Usage

```
colorGraphNodes(graph1, nodes, values,
  colors = c("greenred", "yellowred"))
```

#### **Arguments**

graph1	graphNEL
nodes	vector of node names specifiying which nodes to color. must be same length as parameter foldChanges
values	vector of values indicating fold changes, gene expression values or similar. colors are mapped linearly over the range of these values
colors	string. either "greenred" or "yellowred", specifying which color gradient to use.

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# Value

Returns a graph with specified nodes colored according to the foldChanges

#### Author(s)

Frank Kramer

#### **Examples**

```
# load data and retrieve wnt pathway
  data(biopax2example)
  pwid1 = "pid_p_100002_wntpathway"
  mygraph1 = pathway2RegulatoryGraph(biopax, pwid1)
  mygraph1 = layoutRegulatoryGraph(mygraph1)
# retrieve all nodes
  nodes = nodes(mygraph1)
# random expression data for your nodes
  values = rnorm(length(nodes), mean=6, sd=2)
# color nodes of the graph
  mygraph1 = colorGraphNodes(mygraph1, nodes, values, colors="greenred")
# plot the now colored graph
  plotRegulatoryGraph(mygraph1, layoutGraph=FALSE)
```

createBiopax

This function creates a new Biopax model from scratch

#### **Description**

This function creates a new Biopax model from scratch. This is not necessary if you want to parse a BioPAX export from a file, please see: readBiopax. Returns a biopax model, which is a list with named elements:

```
df The data.frame representing the biopax in Rns_rdf RDF Namespacens_owl OWL Namespacens_bp Biopax Namespacefile NULL
```

# Usage

```
createBiopax(level = 2)
```

#### **Arguments**

level

integer. Specifies the BioPAX level.

diffGraphs 17

### Value

A biopax model

#### Author(s)

Frank Kramer

# **Examples**

```
biopax = createBiopax(level=2)
```

diffGraphs

This function returns the different nodes and edges between graph1 and graph2.

### **Description**

This function returns the different nodes and edges between graph1 and graph2. Layout options of graph1 are kept. Coloring currently not implemented.

# Usage

```
diffGraphs(graph1, graph2, colorNodes = TRUE,
  colors = c("#B3E2CD", "#FDCDAC"))
```

### **Arguments**

graph1 graphNEL graph2 graphNEL colorNodes logical

colors character vector of colors. If colorNodes==TRUE these colors are used for

graph1 and graph2 respectivley.

#### Value

Return the diff between the graphs.

### Author(s)

Frank Kramer

#### **Examples**

```
# load data
data(biopax2example)
pwid1 = "pid_p_100002_wntpathway"
pwid2 = "pid_p_100146_hespathway"
mygraph1 = pathway2RegulatoryGraph(biopax, pwid1)
mygraph2 = pathway2RegulatoryGraph(biopax, pwid2)
plotRegulatoryGraph(diffGraphs(mygraph1,mygraph2))
```

downloadBiopaxData

This function downloads Biopax data from online databases

# Description

This function has an internal list of download links for some online databases. It will retrieve the selected model from the selected database using RCurl. The downloaded file is (if needed) unzipped and ready to be used as input for rBiopaxParser::readBiopax. This function requires package RCurl to run. You can easily skip this step by downloading the exported file yourself and continuing with readBiopax.

#### Usage

```
downloadBiopaxData(database = "NCI",
  model = c("pid", "biocarta", "reactome", "kegg"),
  outputfile = "", version = "biopax2")
```

#### **Arguments**

database string. Select which database you want to download from. Currently only NCI

links have been stored.

model string. Select which model/file you want to download. Currently NCI versions

of the Pathway Interaction Database, Biocarta, Reactome and KEGG are linked.

version string. Select which Biopax Version you want to download.

outputfile string. The file name to save the downloaded data in. If left empty the URL file

name will be used. The unzipped file name can be different from this. Check

the screen output of gunzip.

#### Value

none. Check output for the name of the unzipped biopax .owl file.

#### Author(s)

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#### **Examples**

```
## Not run: file = downloadBiopaxData("NCI", "biocarta", version = "biopax2")
## Not run: biopax = readBiopax(file)
## Not run: biopax
```

generateNewUniqueID

This function generates a new unique id for a biopax model

# Description

This function generates a new unique id for a biopax model. Pass it an startin g point like "pathway" or "protein" to get a niceer looking id.

#### Usage

```
generateNewUniqueID(biopax, id = "")
```

#### **Arguments**

biopax A biopax model

id string. This is used as a prefix for the id.

#### Value

Returns an unused unique ID.

# Author(s)

fkramer

getClassProperties

This function returns the properties of the supplied biopax class.

### **Description**

This function returns the superclasses of the supplied biopax class. It always considers inhertance. Every class inhertis the properties of its super classes. A table listing all available properties and their cardinalities (for Biopax Level 2).

# Usage

```
getClassProperties(classname)
```

#### **Arguments**

classname

A string containing a class name

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### Value

Returns character vector containing the superclasses of the supplied class

### Author(s)

Frank Kramer

### **Examples**

```
getClassProperties("control")
```

getInstanceClass

This function returns the class name of the instance.

# Description

This function returns the class name of the instance.

# Usage

```
getInstanceClass(biopax, id)
```

# Arguments

biopax A biopax model

id string

# Value

Returns the class name of the biopax instance.

# Author(s)

fkramer

# **Examples**

```
# load data
data(biopax2example)
getInstanceClass(biopax, id="ex_m_100650")
```

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getInstanceProperty	This function returns all properties of the specified type for an in-
	stance.

# Description

This function returns all properties of the specified type for an instance. By default this function returns the NAME property of an instance.

### Usage

```
getInstanceProperty(biopax, id, property = "NAME")
```

### **Arguments**

biopax A biopax model

id string

property string. Attention: All properties in Biopax Level 2 are all upper case.

#### Value

Returns a character vector with all properties of the selected type for this instance. Returns NULL if no property of this type is found.

# Author(s)

fkramer

### **Examples**

```
# load data
data(biopax2example)
getInstanceProperty(biopax, id="ex_m_100650", property="NAME")
getInstanceProperty(biopax, id="ex_m_100650", property="ORGANISM")
getInstanceProperty(biopax, id="ex_m_100650", property="COMPONENTS")
```

getNeighborhood This fu

This function returns the neighborhood of a physicalEntity

# Description

This function searches the supplied biopax for interactions that are connected to the molecule or within 'depth' number of steps from it.

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#### Usage

```
getNeighborhood(biopax, id, depth = 1,
 onlyInPathways = c())
```

### Arguments

A biopax model biopax

id string. ID of a physicalEntity (dna, rna, protein, complex, smallMolecule)

depth integer. Search depth, this specifies how far out from the specified molecule the

neighborhood should be streched.

onlyInPathways character vector of pathway IDs. Search only in these pathways for neighbors.

#### Value

Returns ids of interactions within 'depth' number of steps of the specified physicalEntity

#### Author(s)

fkramer

getReferencedIDs This function returns a vector of ids of all instances referenced by the specified instance.

**Description** 

This function takes an id and a biopax model as input. The id of every instance that is referenced is returned. If recursive == TRUE this function recurses through all referenced IDs of the referenced instances and so on. "onlyFollowProperties" limits the recursivness to only certain properties, for example follow only complexes or physicalEntities.

# Usage

```
getReferencedIDs(biopax, id, recursive = TRUE,
 onlyFollowProperties = c())
```

#### **Arguments**

A biopax model biopax

id string. ID of the instance

recursive logical onlyFollowProperties

character vector

getReferencingIDs 23

#### Value

Returns a character vector of IDs referenced by the supplied id in the supplied biopax model.

#### Author(s)

Frank Kramer

#### **Examples**

```
# load data
data(biopax2example)
listComplexComponents(biopax, id="ex_m_100650")
getReferencedIDs(biopax, id="ex_m_100650", recursive=FALSE)
getReferencedIDs(biopax, id="ex_m_100650", recursive=TRUE)
```

getReferencingIDs

This function returns a vector of ids of all instances that reference the supplied id.

### **Description**

This function takes an id and a biopax model as input. The id of every instance that references the supplied id is returned. If recursive == TRUE this function recurses through all referencing IDs of the referencing instances and so on. "onlyFollowProperties" limits the recursivness to only certain properties, for example follow only complexes or physicalEntities.

# Usage

```
getReferencingIDs(biopax, id, recursive = TRUE,
    onlyFollowProperties = c())
```

# **Arguments**

biopax A biopax model

id string. ID of the instance

recursive logical onlyFollowProperties

character vector

#### Value

Returns a character vector of IDs referencing the supplied id in the supplied biopax model.

#### Author(s)

Frank Kramer

24 getSuperClasses

#### **Examples**

```
# load data
data(biopax2example)
listComplexComponents(biopax, id="ex_m_100650")
getReferencingIDs(biopax, id="ex_m_100650", recursive=FALSE)
getReferencingIDs(biopax, id="ex_m_100650", recursive=TRUE)
```

getSubClasses

This function returns the subclasses of the supplied biopax class.

# Description

This function returns the subclasses of the supplied biopax class.

# Usage

```
getSubClasses(classname)
```

#### **Arguments**

classname

A string containing a class name

### Value

Returns character vector containing the subclasses of the supplied class

### Author(s)

Frank Kramer

### **Examples**

```
getSubClasses("control")
```

getSuperClasses

This function returns the superclasses of the supplied biopax class.

### **Description**

This function returns the superclasses of the supplied biopax class.

### Usage

```
getSuperClasses(classname)
```

getXrefAnnotations 25

# Arguments

classname A string containing a class name

#### Value

Returns character vector containing the superclasses of the supplied class

### Author(s)

Frank Kramer

# **Examples**

```
getSuperClasses("control")
```

getXrefAnnotations

This function returns the annotations of the supplied instances.

# **Description**

This function returns the annotations of the supplied IDs in a data.frame.

#### Usage

```
getXrefAnnotations(biopax, id, splitComplexes = FALSE,
  followPhysicalEntityParticipants = TRUE)
```

### **Arguments**

biopax A biopax model

id vector of strings. IDs of instances to get annotations

splitComplexes logical. If TRUE complexes are split up into their components and the annota-

tion of the components is added.

 $follow {\tt Physical Entity Participants}$ 

logical. If TRUE physicalEntityParticipants are resolved to their corresponding

physicalEntities and their annotation is added.

#### Value

Returns data.frame with annotations

#### Author(s)

#### **Examples**

```
# load data
  data(biopax2example)
# no annotations for exactly the complex
getXrefAnnotations(biopax, id="ex_m_100650")
# split up the complex and get annotations for all the molecules involved
getXrefAnnotations(biopax, id="ex_m_100650", splitComplexes=TRUE)
```

hasProperty

Checks if instances in the biopax data.frame have a given property

#### **Description**

Checks if instances in the biopax data.frame have a given property

#### Usage

```
hasProperty(df, property)
```

### **Arguments**

df A data.frame with biopax instances

property A string containing the name of the property to check for

#### Value

Returns TRUE for every row in the data.frame with contains the supplied property. Logical vector with length corresponding to the number of rows in the data.frame.

#### Author(s)

Frank Kramer

internal\_checkArguments

This function checks the supplied arguments if they abid to the given restrictions

# **Description**

This function checks the supplied arguments if they abid to the given restrictions

#### Usage

```
internal_checkArguments(args = c(),
   allowedValues = list(), allowNULL = FALSE,
   allowNA = FALSE, allowEmptyString = TRUE,
   allowInf = TRUE)
```

#### **Arguments**

args The vector of arguments to check

allowedValues A named list of values the argument of a this name is allowed to have

allowNULL Logical, allow NULL or not allowNA Logical, allow NA or not

allowEmptyString

Logical, allow empty strings or not

allowInf Logical, allow values of +/- infinity or not

#### Value

Returns 1 if all checks completed successfully, returns error message otherwise.

#### Author(s)

Frank Kramer

```
\verb|internal_generateXMLfromBiopax| \\
```

This function generates the xmlTree from the supplied biopax model.

#### **Description**

This function is used internally by writeBiopax. It can also be called directly with a fitting dataframe in list(df=data.frame()), but this will probably break things.

#### Usage

```
internal_generateXMLfromBiopax(biopax,
  namespaces = namespaces, verbose = TRUE)
```

#### **Arguments**

biopax A biopax model

namespaces A list of namespaces to use for the generated XML/RDF file

verbose logical

### Value

Returns the xmlTree generated from the supplied biopax model.

### Author(s)

Frank Kramer

 $internal\_getBiopaxModelAsDataFrame$ 

This internal function parses the Biopax XML of the supplied biopax model and returns it in the data.frame format.

# Description

This internal function parses the Biopax XML of the supplied biopax model and returns it in the data.frame format.

### Usage

```
internal_getBiopaxModelAsDataFrame(biopax, biopaxxml,
  verbose = TRUE)
```

### **Arguments**

biopax A biopax object

biopaxxml Biopax XML file read in. See parseBiopax

verbose logical

#### Value

Returns the parsed biopax model in the internal data.frame format.

# Author(s)

Frank Kramer

internal\_NrOfXMLNodes This function in an internal function to count the Number of nodes and child nodes of an XMLNode.

#### **Description**

This function in an internal function to count the Number of nodes and child nodes of an XMLNode.

### Usage

```
internal_NrOfXMLNodes(myXMLNode)
```

### **Arguments**

myXMLNode XMLNode to analyze

#### Value

This function returns the number of Nodes and child Nodes an XMLNode has.

#### Author(s)

Frank Kramer

```
internal_propertyListToDF
```

Internal function to build a data.frame from the list of properties for a new instance

# **Description**

Internal function to build a data.frame from the list of properties for a new instance

# Usage

```
internal_propertyListToDF(class, id, properties,
  namespace_rdf = "rdf")
```

# Arguments

class string. Class name

id string. ID of the instance properties named list of properties.

namespace\_rdf string. This defines the rdf namespace to use.

### Value

Returns a data.frame with the new properties for the given instance

# Author(s)

Frank Kramer

internal\_resolvePhysicalEntityParticipant

This function resolves physicalEntityParticipantIDs to their corresponding physicalEntityIDs

# **Description**

This function resolves physicalEntityParticipantIDs to their corresponding physicalEntityIDs. Every physicalEntityParticipant corresponds exactly to one physicalEntity.

# Usage

```
internal_resolvePhysicalEntityParticipant(biopax,
    physicalEntityId)
```

### **Arguments**

```
\begin{array}{ll} \mbox{biopax} & \mbox{A biopax model} \\ \mbox{physicalEntityId} & \mbox{string. IDs of physicalEntityParticipants to be resolved} \end{array}
```

#### Value

Returns ids of physicalEntity corresponding to the specified physicalEntityParticipantIDs

#### Author(s)

internal\_XMLInstance2DF

This function in an internal function that parses a Biopax Level 2 XMLNode.

# Description

This function in an internal function that parses a Biopax Level 2 XMLNode.

#### Usage

```
internal_XMLInstance2DF(myXMLNode, namespace_rdf)
```

# Arguments

myXMLNode XMLNode

namespace\_rdf String specifying the namespace to use for rdf:resource and rdf:datatype

#### Value

Returns the matrix generated by parsing the XMLNode

# Author(s)

Frank Kramer

intersectGraphs This function returns a graph computed by the insection of supplied graph1 and graph2.

### **Description**

This function returns a graph computed by the insection of supplied graph1 and graph2. Layout and weights of graph1 are kept.

### Usage

```
intersectGraphs(graph1, graph2)
```

# Arguments

graph1 graphNEL graph2 graphNEL

isOfClass

#### Value

Returns the intersection of graph1 and graph2.

#### Author(s)

Frank Kramer

#### **Examples**

```
# load data
data(biopax2example)
pwid1 = "pid_p_100002_wntpathway"
pwid2 = "pid_p_100146_hespathway"
mygraph1 = pathway2RegulatoryGraph(biopax, pwid1)
mygraph2 = pathway2RegulatoryGraph(biopax, pwid2)
plotRegulatoryGraph(intersectGraphs(mygraph1, mygraph2))
```

isOfClass

Checks if instances in the biopax data.frame are of the given class

# **Description**

This function checks if instances in the supplied biopax data.frame are of a given class. If considerInheritance is set to TRUE it also checks if instances are of a given class or any of its inherited classes.

### Usage

```
isOfClass(df, class, considerInheritance = FALSE)
```

# **Arguments**

df A data.frame with biopax instances

class A string containing the class name to check for

considerInheritance

Logical value indicating wether to consider inheritance or not

#### Value

Returns TRUE for every row in the data.frame which is of the supplied class

# Author(s)

Frank Kramer

isOfNamespace 33

isOfNamespace	Check if a classname is preceeded by a certain namespace tag like in "namespace:classname"

# **Description**

This function checks if the supplied input string starts with a supplied namespace tag

#### **Usage**

```
isOfNamespace(classname, namespace = "bp")
```

# **Arguments**

classname A string containing the classname to check namespace A string giving the namespace to check for

#### Value

This function returns TRUE if the supplied classname string is preceded with the supplied namespace string, and FALSE if not.

# Author(s)

Frank Kramer

layoutRegulatoryGraph This function generates a (more or less) beautiful layout for a regulatory graph.

# **Description**

This function generates a (more or less) beautiful layout for a regulatory graph. Call this after you generated a graph with pathway2RegulatoryGraph. Since beauty is always in the eye of the beholder consider this a starting point for making your graphs even nicer. Rgraphviz with dot layout is used. Edges are green/red with normal/tee arrowheads for activations/inhibitions. If you want to specifically paint subgraphs in different colors use lists of vectors with node names for parameter subgraphs and vector of color names for subgraphs.color for your choice of color. The output can be further tweaked by setting layout options using nodeRenderInfo(mygraph) <- list() ... See the Rgraphviz and Graphviz documentations.

#### Usage

```
layoutRegulatoryGraph(mygraph, label = "",
  node.fixedsize = FALSE,
  edge.weights = c("green", "black", "red"),
  edge.arrowheads = c("normal", "tee"),
  subgraphs = list(),
  subgraphs.colors = c("#B3E2CD", "#FDCDAC", "#F4CAE4", "#E6F5C9", "#FFF2AE"))
```

#### **Arguments**

mygraph graphNEL
label Label of the graph
node.fixedsize logical. If font size is fixed or variable in regards to the nodes.
edge.weights vector. which colors to use for weighted edges
edge.arrowheads
vector. which arrowheads to use for weighted edges
subgraphs A list of character vectors with node names defining the sub graphs.
subgraphs.colors

vector. which colors to use for subgraphs

#### Value

Returns the supplied graph in a layouted form with several parameters set for regulatory graph plotting.

#### Author(s)

Frank Kramer

listComplexComponents This function lists all components of a given complex.

#### **Description**

This function returns a (unique) data.frame listing all component IDs, names and classes of the supplied complex.

#### Usage

```
listComplexComponents(biopax, id)
```

#### **Arguments**

biopax A biopax model id string. A complex ID

listInstances 35

#### Value

data.frame

#### Author(s)

Frank Kramer

### **Examples**

```
# load data
  data(biopax2example)
  listComplexComponents(biopax, id="ex_m_100650")
```

listInstances

Lists all instances that conform to the selection criteria.

#### **Description**

Lists all instances that conform to the selection criteria. In contrast to selectInstances this function returns an easier to read list. This function returns an ordered data.frame of class, id and name of the instances. Selection criteria are wether instances belong to a certain class or have the specified id or name. Setting a criteria to NULL ignores this criteria. If includeSubClasses is set to TRUE the class criteria is broadened to include all classes that inherit from the given class, e.g. if class="control" and includeSubClasses=TRUE the function will select catalyses and modulations too, since they are a subclass of class control.

# Usage

```
listInstances(biopax, class = NULL, id = NULL,
name = NULL, includeSubClasses = FALSE)
```

# **Arguments**

biopax A biopax model

class string. Class of the instances to select id string. ID of the instances to select name string. Name of the instances to select

includeSubClasses

logical. If includeSubClasses is set to TRUE the class criteria is broadened to include all classes that inherit from the given class

#### Value

Returns a data.frame containing all instances conforming to the given selection criteria if returnValues=TRUE, only the selector for the internal data.frame otherwise.

#### Author(s)

Frank Kramer

### **Examples**

```
# load data
data(biopax2example)
# list all instances of class "protein"
listInstances(biopax, class="protein")
# list all instances of class "pathway"
listInstances(biopax, class="pathway")
# list all interaction including all subclasses of interactions
listInstances(biopax, class="interaction", includeSubClasses=TRUE)
```

listInteractionComponents

This function lists all components of a given interaction.

#### Description

This function returns a (unique) data.frame listing IDs, names and classes of all components of the supplied interaction.

#### Usage

```
listInteractionComponents(biopax, id,
    splitComplexes = TRUE)
```

#### **Arguments**

biopax A biopax model id string. A complex ID

splitComplexes logical. If TRUE complexes are split up into their components and the added to

the listing.

#### Value

data.frame

#### Author(s)

Frank Kramer

#### **Examples**

```
# load data
data(biopax2example)
listInteractionComponents(biopax, id="ex_i_100036_activator_1")
```

listPathwayComponents This function lists all pathway components of a given pathway.

## Description

This function returns a (unique) data.frame listing all component IDs, names and classes of the supplied pathway.

## Usage

```
listPathwayComponents(biopax, id)
```

## **Arguments**

biopax A biopax model id string. A pathway ID

#### Value

data.frame

## Author(s)

Frank Kramer

# **Examples**

```
# load data
data(biopax2example)
listPathwayComponents(biopax, id="pid_p_100002_wntpathway")
```

listPathways

This function returns a list of all pathway ids.

## **Description**

This function returns a vector of all pathway ids.

# Usage

listPathways(biopax)

## **Arguments**

biopax A biopax model

38 mergePathways

#### Value

Returns a character vector containing the names of all pathways.

## Author(s)

Frank Kramer

## **Examples**

```
# load data
data(biopax2example)
listPathways(biopax)
```

mergePathways

This function merges two given pathways

## **Description**

This function merges two given pathways and appends it to the supplied biopax model. The user has to specify a new name for the pathways and can supply ID, ORGANISM and COMMENT properties for the new pathway. If no ID is supplied, a new unique ID is generated. If no organism property is supplied the organism property of the first pathway is re-used. If ORGANISM is NULL the property is not set. Optionally a comment can be added to the pathway.

#### Usage

```
mergePathways(biopax, pwid1, pwid2, NAME, id = NULL,
    ORGANISM = "", COMMENT = NULL)
```

#### **Arguments**

biopax	A biopax model
pwid1	string. ID of first pathway to merge
pwid2	string. ID of second pathway to merge
NAME	string. Name of the new merged pathway
id	string. ID for the pathway. If NULL a new ID is generated with prefix "pathway".
ORGANISM	string. Organism property of the pathway. By default uses the same organism as the first supplied pathway. If NULL no organism property is set.
COMMENT	string. An optional comment

## Value

A biopax model with the merged pathway added.

## Author(s)

fkramer

```
pathway2AdjacancyMatrix
```

This function generates an adjacency matrix from the activations/inhibitions of a pathway in a biopax model.

#### **Description**

This function internally first calls pathway2RegulatoryGraph, then converts the regulatory graph to an adjacency matrix. See pathway2RegulatoryGraph for more details.

## Usage

```
pathway2AdjacancyMatrix(biopax, pwid,
  expandSubpathways = TRUE, splitComplexMolecules = TRUE,
  useIDasNodenames = FALSE, verbose = TRUE)
```

## **Arguments**

biopax A biopax model

pwid string
expandSubpathways

logical. If TRUE subpathways are expanded into this graph, otherwise only this very pathway is used.

very patnway

splitComplexMolecules

logical. If TRUE every complex is split up into its components. This leads to splitting a single node with name of the complex into several nodes with names of the components, these components all have identical edges.

useIDasNodenames

logical. If TRUE nodes of the graph are named by their molecule IDs instead of using the NAME property. This can help with badly annotated/formatted

databases.

verbose logical

#### Value

Returns the adjacency matrix representing the regulatory graph of the supplied pathway.

#### Author(s)

Frank Kramer

```
# load data
data(biopax2example)
pwid1 = "pid_p_100002_wntpathway"
pwid2 = "pid_p_100146_hespathway"
pathway2AdjacancyMatrix(biopax, pwid1)
```

pathway2Geneset

This function generates the gene set of a pathway.

#### **Description**

This function generates a gene set of all physicalEntity's of a pathway. First all interactions of the pathway are retrieved and all components of these interactions are then listed.

## Usage

```
pathway2Geneset(biopax, pwid)
```

#### **Arguments**

biopax A biopax model

pwid string

#### Value

Returns the gene set of the supplied pathway.

#### Author(s)

Frank Kramer

#### **Examples**

```
# load data
  data(biopax2example)
  pwid1 = "pid_p_100002_wntpathway"
  pathway2Geneset(biopax, pwid=pwid1)
```

pathway2RegulatoryGraph

This function generates the regulatory graph from the activations/inhibitions of a pathway in a biopax model.

#### **Description**

This functions builds a graph from the pathway components of the supplied pathway. Only instances of class 'control' are considered, this leads a functinal graph with all edges either representing activations or inhibitions. No transports, no translocation, etc. If desired complexes can be split up into several nodes, this can sometimes lead to a more complex and cluttered graph. There can not be multiple edges between 2 nodes. Whenever duplicated edges are generated (especially by splitting up complexes) a warning is thrown.

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#### Usage

```
pathway2RegulatoryGraph(biopax, pwid,
  expandSubpathways = TRUE, splitComplexMolecules = TRUE,
  useIDasNodenames = FALSE, verbose = TRUE)
```

#### **Arguments**

biopax A biopax model

pwid string
expandSubpathways

logical. If TRUE subpathways are expanded into this graph, otherwise only this

very pathway is used.

splitComplexMolecules

logical. If TRUE every complex is split up into its components. This leads to splitting a single node with name of the complex into several nodes with names

of the components, these components all have identical edges.

useIDasNodenames

logical. If TRUE nodes of the graph are named by their molecule IDs instead of using the NAME property. This can help with badly annotated/formatted

databases.

verbose logical

#### Value

Returns the representing the regulatory graph of the supplied pathway in a node-edge-list graph.

#### Author(s)

Frank Kramer

## **Examples**

```
# load data
data(biopax2example)
pwid1 = "pid_p_100002_wntpathway"
pwid2 = "pid_p_100146_hespathway"
mygraph = pathway2RegulatoryGraph(biopax, pwid1)
plotRegulatoryGraph(mygraph)
```

plotRegulatoryGraph

This function layouts a regulatory graph and plots it using Rgraphviz.

# Description

This function takes a regulatory graph as generated by pathway2regulatoryGraph and plots it using standard layout options of layoutRegulatoryGraph. This function is a wrapper for layoutRegulatoryGraph with standard parameters. Subgraphs can be painted with different colors. This can be done by passing parameter subgraph a list of character vectors with node names.

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## Usage

```
plotRegulatoryGraph(mygraph, subgraphs = list(),
  layoutGraph = TRUE)
```

## **Arguments**

mygraph graphNEL, regulatory graph

subgraphs list of character vectors with node names

layoutGraph logical. If FALSE the graph is not laid out again but send directly to Rgraphviz::renderGraph.

## Value

none

## Author(s)

Frank Kramer

## **Examples**

```
# load data
data(biopax2example)
pwid1 = "pid_p_100002_wntpathway"
pwid2 = "pid_p_100146_hespathway"
mygraph = pathway2RegulatoryGraph(biopax, pwid1)
plotRegulatoryGraph(mygraph)
```

print.biopax

Print a biopax object.

## Description

Print a biopax object.

## Usage

```
## S3 method for class 'biopax'
print(x, ...)
```

# Arguments

x A biopax object to print.

... Other arguments to be passed to print.

```
data(biopax2example)
  print(biopax)
```

readBiopax 43

readBiopax

This function reads in a Biopax .owl file

## Description

This function reads in a Biopax .owl file and generates the internal data.frame format used in this package. This function can take a while with really big Biopax files like NCIs Pathway Interaction Database or Reactome. In almost every case this is your starting point. Returns a biopax model, which is a list with named elements:

```
df The data.frame representing the biopax in Rns_rdf RDF Namespacens_owl OWL Namespace
```

ns\_bp Biopax Namespace

file File name

## Usage

```
readBiopax(file, verbose = TRUE)
```

# Arguments

file string. File name

verbose logical. Output messages about how parsing is going and so on.

#### Value

A biopax model

## Author(s)

Frank Kramer

```
## Not run: biopax = readBiopax(file="biopaxmodel.owl")
## Not run: biopax
```

removeProperties

removeInstance

This function removes an instance

## **Description**

This function removes an instance from an existing biopax model.

## Usage

```
removeInstance(biopax, id)
```

## Arguments

biopax A biopax model

id string. ID of the instance

#### Value

Returns the supplied biopax model with the instance removed from it.

## Author(s)

Frank Kramer

removeProperties

This function removes a property

## **Description**

This function removes a property fram an existing biopax instance.

## Usage

```
removeProperties(biopax, id, properties)
```

## **Arguments**

biopax A biopax model

id string. ID of the instance

properties character vector. listing the properties to remove.

# Value

Returns the supplied biopax model with properties removed from this instance.

## Author(s)

selectInstances 45

selectInstances

Returns all instances that conform to the selection criteria.

#### **Description**

Returns all instances that conform to the selection criteria. This function returns a subset of the internal data.frame of the biopax object. Selection criteria are wether instances belong to a certain class or have the specified id, property or name. Setting a criteria to NULL ignores this criteria. If returnValues is set to FALSE only the selector (a logical vector with length of the internal data.frame) is returned, otherwise the selected data is returned. If includeSubClasses is set to TRUE the class criteria is broadened to include all classes that inherit from the given class, e.g. if class="control" and includeSubClasses=TRUE the function will select catalyses and modulations too, since they are a subclass of class control. If includeReferencedInstances is set to TRUE all instances that are being referenced by the selected instances are being selected too. The parameter works recursively, this means for example that a selected pathway and all it's interactions, complexes, molecules and annotations are returned if this parameter is set to true. This parameter is especially helpful if you want to migrate or merge knowledge from different data bases.

#### Usage

```
selectInstances(biopax, class = NULL, id = NULL,
    property = NULL, name = NULL, returnValues = TRUE,
    includeSubClasses = FALSE,
    includeReferencedInstances = FALSE)
```

## **Arguments**

biopax A biopax model

class string. Class of the instances to select id string. ID of the instances to select

property string. Return only this property of the instances

name string. Name of the instances to select

returnValues logical. If returnValues is set to FALSE only the selector (a logical vector with

length of the internal data.frame) is returned, otherwise the selected data is re-

turned

includeSubClasses

logical. If includeSubClasses is set to TRUE the class criteria is broadened to

include all classes that inherit from the given class

include Referenced Instances

logical. If includeReferencedInstances is set to TRUE all instances that are being referenced by the selected instances are being selected too

#### Value

Returns a data.frame containing all instances conforming to the given selection criteria if returnValues=TRUE, only the selector for the internal data.frame otherwise.

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#### Author(s)

Frank Kramer

#### **Examples**

```
# load data
data(biopax2example)
# select the subset of the internal data.frame that belongs to class "protein"
selectInstances(biopax, class="protein")
# select the subset of the internal data.frame that belongs to class "interaction"
selectInstances(biopax, class="interaction")
# select the subset of the internal data.frame that belongs to class "interaction" or any of its sub classes, like of selectInstances(biopax, class="interaction", includeSubClasses=TRUE)
# select the subset of the internal data.frame that belongs to class "pathway" AND is a "NAME" property
selectInstances(biopax, class="pathway", property="NAME")
```

splitComplex

This functions splits up a complex into its components.

#### **Description**

This function looks up the supplied Complex ID and returns the names of all its components.

#### **Usage**

```
splitComplex(biopax, complexid, recursive = TRUE)
```

#### **Arguments**

biopax A biopax model

complexid string ID of an complex

recursive logical

## Value

Returns a character vector with the names of all subcomponents.

#### Author(s)

Frank Kramer

```
# load data
data(biopax2example)
selectInstances(biopax, id="ex_m_100650")
listInstances(biopax, id="ex_m_100650")
listComplexComponents(biopax, id="ex_m_100650")
splitComplex(biopax, complexid="ex_m_100650")
```

striphash 47

striphash

Strips a hash in front of a string

## Description

Strips a hash in front of a string

## Usage

striphash(x)

## **Arguments**

Χ

A string to be stripped off a preceeding hash

## Value

The supplied string with a hash "#" stripped off front.

## Author(s)

Frank Kramer

stripns

Strips a namespace tag off a supplied classname string

## Description

Strips a namespace tag off a supplied classname string

## Usage

```
stripns(classname)
```

## Arguments

classname

A string containing a classname preceded by a namespace tag

## Value

The classname with the namespace tag stripped off it.

## Author(s)

48 transitiveReduction

transitiveClosure

This function generates the transitive closure of the supplied graph.

## **Description**

This function generates the transitive closure of the supplied graph. In short: if A->B->C then an edge A->C is added. Edge weights are conserved if possible (in a hopefully smart way).

## Usage

```
transitiveClosure(mygraph)
```

#### **Arguments**

mygraph

graphNEL

#### Value

Returns the transitive closure of the supplied graph.

#### Author(s)

Frank Kramer

transitiveReduction

This function generates the transitive reduction of the supplied graph.

## **Description**

This function generates the transitive reduction of the supplied graph. In short: if A->B->C AND A->C then edge A->C is removed. Edge weights are conserved if possible (in a hopefully smart way).

## Usage

```
transitiveReduction(mygraph)
```

#### **Arguments**

mygraph

graphNEL

#### Value

Returns the transitive reduction of the supplied graph.

## Author(s)

unfactorize 49

unfactorize

Replace factors/levels in a data.frame and use plain strings instead

## **Description**

This function takes a data.frame as argument and returns it with strings instead of factors.

## Usage

```
unfactorize(df)
```

## Arguments

df

any data.frame with factor levels in at least one column

#### Value

The data.frame is returned using strings instead of factors.

## Author(s)

Frank Kramer

uniteGraphs

This function unites two graphs.

## **Description**

This function unites the two supplied graphs. Layout parameters from graph1 are used. If colorN-odes==TRUE the returned graph has different colors for overlapping nodes and nodes individual for each graph.

## Usage

```
uniteGraphs(graph1, graph2, colorNodes = TRUE,
colors = c("#B3E2CD", "#FDCDAC", "#F4CAE4"))
```

#### **Arguments**

graph1 graphNEL graph2 graphNEL colorNodes logical

colors colors character vector of colors. If colorNodes==TRUE these colors are used

for graph1 and graph2 respectivley.

50 writeBiopax

#### Value

Return a graph generated by uniting the two supplied graphs

#### Author(s)

Frank Kramer

#### **Examples**

```
# load data
data(biopax2example)
pwid1 = "pid_p_100002_wntpathway"
pwid2 = "pid_p_100146_hespathway"
mygraph1 = pathway2RegulatoryGraph(biopax, pwid1)
mygraph2 = pathway2RegulatoryGraph(biopax, pwid2)
plotRegulatoryGraph(uniteGraphs(mygraph1,mygraph2))
```

writeBiopax

This function writes out a biopax model.

#### **Description**

This function writes out a biopax model, as generated by readBiopax, to either a file or returns the xmlTree if file is omitted.

# Usage

```
writeBiopax(biopax, file = "", verbose = TRUE,
  overwrite = FALSE,
namespaces = list(rdf = "http://www.w3.org/1999/02/22-rdf-syntax-ns#", bp = "http://www.biopax.org/
```

## **Arguments**

biopax A biopax model as generated by readBiopax

file A string giving a file name.

verbose logical

overwrite logical, if TRUE an already existing file will be overwritten, otherwise an error

is thrown

namespaces A list of namespaces to use for the generated XML/RDF file

#### Value

Returns the xmlTree object generated from the biopax model. If a filename is supplied the XML is written to this file.

## Author(s)

writeBiopax 51

```
# load data
data(biopax2example)
## Not run: writeBiopax(biopax, file="mybiopax.owl")
```

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