

# Multipath - an R package to create integrated reproducible multilayered pathway models

true

2023-03-15

## Introduction

Biological pathway data integration has become a topic of interest in the past years. This interest originates essentially from the continuously increasing size of existing prior knowledge as well as from the many challenges scientists face when studying biological pathways. Multipath is a framework that aims at helping re-trace the use of specific pathway knowledge in specific publications, and easing the data integration of multiple pathway types and further influencing knowledge sources. Using Multipath, BioPax-encoded pathways can be parsed and embedded into multilayered graphs. Modifications can be applied to these graphs to generate different views. The package is implemented as a part of the Multipath Project directed by Dr. Frank Kramer .

## Installation

### Preinstallation

Multipath depends on multiple packages. The packages are the following: UniProt.ws, dbparser, rBiopaxParser, mully, TCGAretreiver, stringr, svMisc, uuid, dplyr, crayon Please make sure to install the packages UniProt.ws,rBiopaxParser and mully before using the package.

To install the UniProt.ws package:

```
if (!requireNamespace("BiocManager", quietly = TRUE))  
  install.packages("BiocManager")
```

```
BiocManager::install("UniProt.ws")
```

To install the mully package:

```
require(devtools)  
install_github("frankkramer-lab/mully")  
library(mully)
```

To install the rBiopaxParser package:

```
require(devtools)  
install_github("frankkramer-lab/rBiopaxParser")  
library(rBiopaxParser)
```

## Installation via Github

```
require(devtools)
install_github("frankkramer-lab/Multipath")
library(Multipath)
```

## Available Functions

### addDBLayer

#### Add a drug layer to a mully graph

This function is used to add a DrugBank layer to an existing mully model. The function needs the following arguments:

- **g** - The mully graph
- **drugList** - The list of DrugBank Ids of the drugs to be added. This argument can be either a string (one drug) or a list of strings (multiple drugs)
- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`

The function returns a mully graph with the added drug layer

#### *Example*

```
g=mully("DrugBank",direct=T)
data=loadDBXML(DrugBankFile)
g=addDBLayer(g,data,c("DB00001","DB06605"))
```

### addDiseaseLayer

**Add OMIM Layer with its respective Nodes and Edges** The function first extracts the proteins available in a Mully graph. Then, the proteins are queried from the UPKB database to check if they have a cross-reference to OMIM. The proteins, along with their returned OMIM ids, are then returned as a data frame, which is subsequently fed into another function to check if the returned OMIM ids also have a reference to the same protein. Finally, a new Disease layer is added to the Mully graph and edges are created between OMIM ids and proteins if a connection is proven to be true. The same process is repeated with Kegg genes to also create edges between the OMIM ids and the genes. Please note that the function should be preceded by calling `romim::set_key('KEY')`. The KEY could be requested via OMIM's official website. The function needs the following arguments:

- **g** - The mully graph - must contain a protein layer
- **biopax** - The BioPaX object containing the parsed data from an OWL file. This can be obtained using `readBiopax(filepath)`

#### *Example*

```
biopax=readBiopax("wnt.owl")
pathwayID=listPathways(biopax)$id[1]
g=Multipath::pathway2Mully(biopax,pathwayID)
g=addDiseaseLayer(g,biopax)
```

## addGenesLayer

**Add KEGG Gene Layer with its respective Nodes and Edges** The function first extract the proteins available on a mully graph. Then the protein are queried from UPKB database to check if they have a cross-reference to KEGG. Afterwards the proteins along with their returned genes are returned into a data frame that is then feed into another function to check if the returned genes also have a reference to that same protein. After all, a new genes layer is added to the Mully graph and edges are added between genes and protein if a connection is proven true. The function needs the following arguments:

- **g** - The mully graph - must contain a protein layer
- **biopax** - The BioPaX object containing the parsed data from an OWL file. This can be obtained using `readBiopax(filepath)`

### *Example*

```
biopax=readBiopax("wnt.owl")
pathwayID=listPathways(biopax)$id[1]
g=Multipath::pathway2Mully(biopax,pathwayID)
g=addGenesLayer(g,biopax)
```

## addStep

### Track a modification of a graph

The function saves a modification applied to a mully graph. It applies the step to the graph and saves the modification step in the pathwayView Object. Not all of the arguments are mandatory, they depend on the step that has to be applied. The function needs the following arguments:

- **v** - The input view in which the modification should be saved
- **action** - The type of action to be applied. Can either be “add” or “remove”
- **element** - The type of the element to be modified. Can either be “node”, “edge”, or “layer”
- **name** - The name of the element to be modified. This argument is only mandatory for nodes and edges
- **layername** - The layer name. This argument is only mandatory for action “add” and element “node”
- **V1** - The start node of an edge. This argument is only mandatory for element “edge”
- **V2** - The end node of an edge. This argument is only mandatory for element “edge”
- **attributes** - The named list of attributes of the element. This argument is required only for action “add”. It is optional for both elements “node” and “edge”, but mandatory if the edge already exists
- **multi** - A boolean whether to select multi-edges or not. This is only mandatory for action “remove” and element “edge”. By default set to FALSE, in which case the attributes of the specified edge should be given
- **trans** - A boolean whether to add transitive edges upon removal of nodes or layers

The function returns the view with the added step. *Example*

```
g=mully::demo()
view=pathwayView(g,"View1")
view=addStep(view,"remove","layer","disease")
```

## addUPKBLayer

### Add a protein layer to a mully graph

This function is used to add a UniProt protein layer to an existing mully model. The function needs the following arguments: - **g** - The mully graph - **up** - The UniProt.ws Object - **proteinList** - The list of UniProt Ids of the proteins to be added - **col** - The list of attributes associated to the UniProtKB Entries to be retrieved

The function returns the mully graph with the added UniProt layer The function should be preceded by `UniProt.ws()` to get the UniProt.ws Object

#### *Example*

```
up=UniProt.ws()
g=mully("UniProt")
g=addUPKBLayer(g,up,proteinList=c("P02747","P00734","P07204"),col=c("UNIPROTKB","PROTEIN-NAMES"))
```

## downloadPathway

### Download Reactome Pathways in BioPAX level 2 and 3

This function is used to download one or a list of pathways, encoded in BioPAX level 2 or 3. The function needs the following arguments:

- **pathwayID** - The Reactome ID or list of IDs of the pathways to be downloaded. The ID should start with R-HSA-.
- **biopaxLevel** - The BioPAX Level, 2 or 3. By default set to 3.
- **destDirectory** - The Directory in which the Pathway Files should be saved. If missing, the files are saved in the working directory. The Reactome IDs are used to name the files.
- **overwrite** - A Boolean whether to overwrite existing files with the same name.

The function returns the path to the directory in which the files are downloaded.

#### *Example*

```
downloadPathway(c("R-HSA-195721","R-HSA-9609507"),biopaxLevel=3,overwrite=T)
```

## getAllUPKB

### Get all proteins' entries from UniProt

The function is used to fetch all protein entries from UniProt. The function needs the following arguments: - **up** - The UniProt.ws Object

The function returns a dataframe containing the Protein's entries with the ID and Name.

Should be preceded by `UniProt.ws()` to get the UniProt.ws Object

#### *Example*

```
up=UniProt.ws()
allProteins=getAllUPKB(up)
```

## getDBCarriers

### Get the Carriers Protein Targets of given DrugBank drugs

Protein Targeted by Drugs are divided in DrugBank into 4 types: Targets, Enzymes, Carriers and Transporters. This function is used to extract the carriers from the dataframe containing the information on the drugs parsed from the DrugBank XML File.

The function needs the following arguments:

- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **drugList** - The list of DrugBank Ids of the drugs. This argument can be either a string (one drug) or a list of strings (multiple drugs)

The function returns a dataframe containing all information on the carriers targeted by the given drug list.

#### *Example*

```
data=loadDBXML(DrugBankFilePath)
getDBCarriers(data,"DB00001")
```

## getDBDrug

### Get DrugBank drug entry

This function extracts information on one or a list of Drugs from the dataframe parsed from the DrugBank XML file. The function needs the following arguments:

- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **drug** - The ID or list of IDs of the DrugBank drug entries starting with “DB”

This function returns a dataframe containing the DrugBank entry with its information

#### *Example*

```
data=loadDBXML(DrugBankFilePath)
getDBDrug(data,"DB00001")
```

## getDBDrugInteractions

**Get DrugBank Drug to Drug Interactions** This function is used to extract Drug Interactions from the dataframe containing the information on the Drug in DrugBank, parsed from the downloaded XML File.

The function needs the following arguments:

- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **drug** - The ID of the DrugBank drug entry starting with “DB”. This argument can be either a string (one drug) or a list of strings (multiple drugs).

The function returns a dataframe containing the DrugBank interactions in which the given drug is involved

#### *Example*

```
data=loadDBXML(DrugBankFilePath)
getDBDrugInteractions(data,"DB06605")
```

## getDBEnzymes

### Get the Enzyme Protein Targets of given DrugBank drugs

Protein Targeted by Drugs are divided in DrugBank into 4 types: Targets, Enzymes, Carriers and Transporters. This function is used to extract the enzymes from the dataframe containing the information on the drugs parsed from the DrugBank XML File.

The function needs the following arguments:

- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **drugList** - The list of DrugBank Ids of the drugs. This argument can be either a string (one drug) or a list of strings (multiple drugs)

The function returns a dataframe containing all information on the enzymes targeted by the given drug list.

#### *Example*

```
data=loadDBXML(DrugBankFilePath)
getDBEnzymes(data,"DB00001")
```

## getDBTargets

### Get the Target Protein Targets of given DrugBank drugs

Protein Targeted by Drugs are divided in DrugBank into 4 types: Targets, Enzymes, Carriers and Transporters. This function is used to extract the targets from the dataframe containing the information on the drugs parsed from the DrugBank XML File.

The function needs the following arguments:

- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **drugList** - The list of DrugBank Ids of the drugs. This argument can be either a string (one drug) or a list of strings (multiple drugs)

The function returns a dataframe containing all information on the targets of the given drug list.

#### *Example*

```
data=loadDBXML(DrugBankFilePath)
getDBTargets(data,"DB00001")
```

## getDBTransporters

### Get the Transporters Protein Targets of given DrugBank drugs

Protein Targeted by Drugs are divided in DrugBank into 4 types: Targets, Enzymes, Carriers and Transporters. This function is used to extract the transporters from the dataframe containing the information on the drugs parsed from the DrugBank XML File.

The function needs the following arguments:

- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFilePath)`
- **drugList** - The list of DrugBank Ids of the drugs. This argument can be either a string (one drug) or a list of strings (multiple drugs)

The function returns a dataframe containing all information on the transporters targeted by the given drug list.

#### *Example*

```
data=loadDBXML(DrugBankFilePath)
getDBTransporters(data,"DB00001")
```

## getDBtoUPKB

### Get DrugBank Drugs to UniProt Proteins Relations from DrugBank

This function is used to extract Drug Targets from the dataframe containing the information on the drugs parsed from the DrugBank XML File. It merges the targets returned by 4 functions: enzymes, targets, transporters and carriers. The function needs the following arguments:

- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **drugList** - The list of DrugBank Ids of the drugs. This argument can be either a string (one drug) or a list of strings (multiple drugs)
- **proteinList** - The list of UniProt Ids of the proteins

The function returns a dataframe containing the connections between DrugBank drugs and UniProt proteins retrieved from DrugBank.

#### *Example*

```
data=loadDBXML(DrugBankFilePath)
getDBtoUPKB(data,c("DB00001","DB00002","DB00006"),c("P02747","P00734","P07204","P05164"))
```

## getKeggGene

**Get A Gene using KEGGREST package** The function is used to query the KEGGGenes database and receive all available information regarding a specific gene. The list of genes should be provided. Since KEGGGenes API only allows for 10 entries per query, this function split the input into a lists of 10 elements. The function needs the following arguments:

- **geneList** - The List of genes to query from KEGGGenes

#### *Example*

```
geneList=c("hsa:122706","hsa:4221","hsa:8312")
genes = getKeggGene(geneList)
```

## getKEGGtoDATABASE

**Get KEGG Genes to a cross-reference from KEGG** The function is used to query gene entries from KEGG Genes that have a cross reference to another database which include either “UniProtKB” or “OMIM” or “Ensembl”. The function needs the following arguments:

- **dbName** - The name of the cross reference of interest. The allowed input value is : “Uniprot”, “Omin” or “Ensembl”. The function does not differentiate between upper and lower case.
- **geneList** - The list of KEGGGenes of interest.

### *Example*

```
getKEGGtoDATABASE("UniProt",c("hsa:122706","hsa:4221","hsa:8312"))
```

## getKEGGtoOMIM

**Get KEGG Genes that has OMIM as a cross-reference from KEGGGenes** The function is used to query gene entries from KEGG Genes that have a cross reference to “OMIM” The function needs the following arguments:

- **geneList** - The list of KEGGGenes of interest.

### *Example*

```
getKEGGtoOMIM(c("hsa:122706","hsa:4221","hsa:8312"))
```

## getKeggUpkbRelations

**Gets genes and proteins that are referenced to each other** The function relies on two other functions: `getRelatedGenes(g,biopax)` and `getKEGGtoDatabase(dbName,geneList)` to find and return genes and proteins that are related to each other as a dataframe. The function needs the following arguments:

- **g** - The Mully graph. The graph should contain a protein layer.
- **biopax** - The bioPax object.

### *Example*

```
up = UniProt.ws()
biopax=readBiopax("wnt.owl")
pathwayID=listPathways(biopax)$id[1]
g=Multipath::pathway2Mully(biopax,pathwayID)
g=addGenesLayer(g,biopax)
getUPKBtoKEGG(g, biopax)
```



## getKeggOmimRelation

**Gets the genes and diseases that are referenced to each other** This function finds the relation between the available Genes that are extracted from the mully graph and their respective “OMIM” cross reference. The function depends on two functions: `getKEGGtoOMIM(geneList)` and `getOmimToKEGG(omimIds)`. A data frame is returned with all information about the genes and their cross reference “OMIM”. Please note that the function should be preceded by by calling `romim::set_key('KEY')`. The KEY could be requested via OMIM’s official website. The function needs the following arguments:

- **g** - The Mully graph. The graph should contain a “KEGGGENES” layer.
- **biopax** - The bioPax object.

### *Example*

```
up = UniProt.ws()
biopax=readBiopax("wnt.owl")
pathwayID=listPathways(biopax)$id[1]
g=Multigraph::pathway2Mully(biopax,pathwayID)
g=addGenesLayer(g,biopax)
getKeggOmimRelation(g,biopax)
```

## getOmimToUPKB

**Get Omim to UniprotKB relations from OMIM** This function is used to query OMIM entries that have a cross-reference to “UniProtKB” proteins. Please note that the function should be preceded by by calling `romim::set_key('KEY')`. The KEY could be requested via OMIM’s official website. The function needs the following arguments:

- **omimIds** - The list of Omim ids

### *Example*

```
getOmimToUPKB(c("611137", "613733", "603816"))
```

## getOmimToKEGG

**Get Omim to KEGG Genes relations from OMIM** This function is used to query OMIM entries that have a cross-reference to “KEGG Genes”. Please note that the function should be preceded by by calling `romim::set_key('KEY')`. The KEY could be requested via OMIM’s official website. The function needs the following arguments:

- **omimIds** - The list of Omim ids

### *Example*

```
getOmimToKEGG(c("611137", "613733", "603816"))
```

## getRelatedGenes

**Get proteins that has a reference to KEGG Genes from a mully graph and a biopax object** The function first retrieves all the proteins available on a protein layer in a mully graph. The proteins are then queried using the function `getUPKBInfo()` to find the genes that are cross referenced to the proteins. The function returns a data frame containing : Uniprot ID, KEGG ID, the graph's internal ID and the source. The function needs the following arguments:

- **g** - The Mully graph. The graph should contain a protein layer.
- **biopax** - The bioPax object.

### *Example*

```
up = UniProt.ws()
biopax=readBiopax("wnt.owl")
pathwayID=listPathways(biopax)$id[1]
g=Multipath::pathway2Mully(biopax,pathwayID)
g=addGenesLayer(g,biopax)
getRelatedGenes(g, biopax)
```

## getPathwayID

### **Get internal pathway ID in a BioPAX file**

This function is used to get the internal ID of a pathway in a parsed BioPAX object. A BioPAX file can contain multiple pathways, indexed internally using ID starting with "Pathway" followed by the number of the pathway. Each pathway in the file has a Reactome and an internal ID. The latter can be extracted using this function. This should be preceded by `readBiopax(filepath)` to obtain the biopax object The function needs the following arguments:

- **biopax** - The biopax object
- **reactomeID** - The Reactome ID of the pathway

The function returns the internal ID of the pathway in the parsed BioPAX object.

### *Example*

```
biopax=readBiopax("pi3k.owl")
id=getPathwayID(biopax,"R-HSA-167057")
pi3kmully=pathway2mully(biopax,id)
```

## getUPKBDBRelations

### **Get Protein and Drugs relations from UniProt and DrugBank**

The function is used to obtain drug targets from UniProt and DrugBank. It combines the returned relations from both functions `getDBtoUPKB` and `getUPKBtoDB`. The function needs the following arguments:

- **up** - The UniProt.ws Object
- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **proteinList** - The list of UniProt Ids of the proteins

- **drugList** - The list of DrugBank Ids of the drugs. This argument can be either a string (one drug) or a list of strings (multiple drugs)

The function returns a dataframe containing the connections between DrugBank drugs and UniProt proteins retrieved from DrugBank and UniProt. The function should be preceded by:

1. `UniProt.ws()` to get the UniProt.ws Object
2. `loadDBXML(DrugBankFile)` to get the argument data

### *Example*

```
up=UniProt.ws()
data=loadDBXML(DrugBankFilePath)
relations=getUPKBDBRelations(up,data,proteinList=c("P02747","P07204"),drugList=c("DB00001","DB00006"))
```

## getUPKBInfo

### Get Proteins from UniProtKB

The function is used to fetch information on a list of protein entries from UniProt. The function needs the following arguments: - **up** - The UniProt.ws Object - **proteins** - The list of UniProtKB Proteins ID to be retrieved - **col** - The list of attributes associated to the UniProtKB Entries to be retrieved

The function returns a dataframe containing the protein entries with the selected attributes. To get the list of possible columns, you can call `columns(UniProt.ws())`. The function should be preceded by `UniProt.ws()` to get the UniProt.ws Object.

### *Example*

```
up <- UniProt.ws()
getUPKBInfo(up,c("Q6ZS62","P14384","P40259"),c("PROTEIN-NAMES","DRUGBANK","GO","REACTOME"))
```

## getUPKBInteractions

### Get the interactions of given proteins from UniProt

The function is used to fetch interactions between proteins from the UniProt Database. The function needs the following arguments:

- **up** - The UniProt.ws Object
- **proteins** - The list of proteins of which the interactions should be retrieved

The function returns a dataframe containing the interactions between the given proteins. The function should be preceded by `UniProt.ws()` to get the UniProt.ws Object.

### *Example*

```
up=UniProt.ws()
interactions=getUPKBInteractions(up,c("P02747","P07204","P00734"))
```

## getUPKBtoKEGG

### Get Proteins from UniProtKB that has KEGG as a cross reference

The function is used to fetch information on a list of protein entries from UniProt. It returns a dataframe showing the protein and its respective KEGG id if it could be located as a cross reference. The function needs the following arguments:

- **up** - The UniProt.ws Object
- **proteinList** - The list of UniProtKB Proteins ID to be retrieved
- **geneList** - This is an optional argument. It can be used to show the proteins that only has cross reference to any element in the gene list. If not provided, a dataframe with all fetched information about the protein along with their cross reference being KEGG is returned.

The function should be preceded by `UniProt.ws()` to get the UniProt.ws Object.

#### *Example*

```
up = UniProt.ws()
proteinList = c("P02747", "P00734", "P07204", "A0A0S2Z4R0", "O15169")
geneList=c("hsa:122706", "hsa:4221", "hsa:8312")
getUPKBtoKEGG(up, geneList, proteinList)
```

## getUPKBRelatedDiseases

**Get proteins that has a reference to OMIM from a mully graph and a biopax object** The function first retrieves all the proteins available on a protein layer in a mully graph. The proteins are then queried using the function `getUPKBInfo()` to find the OMIM ids that are cross referenced to the proteins. The function returns a data frame containing : Uniprot ID, OMIM ID, the protein's internal ID and the source. Please note that the function should be preceded by by calling `romim::set_key('KEY')`. The KEY could be requested via OMIM's official website. The function needs the following arguments:

- **g** - The Mully graph. The graph should contain a protein layer.
- **biopax** - The bioPax object. *Example*

```
biopax=readBiopax("wnt.owl")
pathwayID=listPathways(biopax)$id[1]
g=MultiPath::pathway2Mully(biopax, pathwayID)
g=getUPKBRelatedDiseases(g, biopax)
```

## getUPKBtoDB

### Get UniProt Proteins to DrugBank Drugs relations from UniProt

This function is used to fetch relations between a list of proteins and a list of drugs from the UniProt Database. The function needs the following arguments:

- **up** - The UniProt.ws Object
- **proteinList** - The list of UniProt Ids of the proteins
- **drugList** - The ID of the DrugBank drug entry starting with "DB". This argument can be either a string (one drug) or a list of strings (multiple drugs).

The function returns a dataframe containing the connections between UniProt proteins and DrugBank drugs retrieved from UniProt. The function should be preceded by `UniProt.ws()` to get the UniProt.ws Object.

### *Example*

```
up=UniProt.ws()
getUPKBtoDB(up,c("P02747","P00734","P07204"),c("DB00001","DB00002"))
```

## interactionKegg

**Interaction between KEGG genes and other databases** Get interactions between a KEGG gene input and all the databases - returns NA when there is no cross reference to other databases. The function should be preceded by `transformKeggData(list_keggGet, list_Get)` The function needs the following arguments:

- **keggInput** - The dataframe returned by the function `transformKeggData(list_keggGet, list_Get)`

### *Example*

```
geneList=c("hsa:122706","hsa:4221","hsa:8312")
genes = getKeggGene(geneList)
genesinteraction = interactionKegg(genes)
```

## loadDBXML

### **Load DrugBank XML file**

This function is used to read and parse the file downloaded from the DrugBank Database containing the complete information on the drug entries. The function needs the following argument:

- **file** - The path to the DrugBank XML file. This can be downloaded from the DrugBank official Website ([drugbank.ca](http://drugbank.ca)). An account with an institutional e-mail is required.

This function returns a dataframe containing the parsed information from DrugBank. This can be used to extract any additional information on the DrugBank entries

This function should be called before using any function to query the DrugBank database. Since the parsing of DrugBank takes time, this function should only be called once.

### *Example*

```
data=loadDBXML(DrugBankFilePath)
```

## multipath

### **Generate Multipath Graph from General Data**

This function is used to generate a mully graph from a list of drugs and proteins. The function creates a multilayered graph with a drug and protein layer, and adds the inter- and intractions to it. The function needs the following arguments:

- **name** - The name of the graph to be generated
- **up** - The `Uniprot.ws()` object

- **proteinList** - The list of proteins of which the interactions should be retrieved
- **data** - The dataframe containing the parsed information of DrugBank. This argument can be obtained using the function `loadDBXML(DrugBankFile)`
- **drugList** - The list of DrugBank Ids of the drugs. This argument can be either a string (one drug) or a list of strings (multiple drugs)

The function returns a mully graph with the added data. The function should be preceded by:

1. `UniProt.ws()` to get the UniProt.ws Object
2. `loadDBXML(DrugBankFile)` to get the argument data

### *Example*

```
up=UniProt.ws()
data=loadDBXML(DrugBankFilePath)
g=multipath(up=up,proteinList=c("P02747","P05164"),data=data,drugList=c("DB00001","DB00006"))
```

## pathway2Mully

**Build a mully graph from a given pathway** This function builds a multilayered mully graph of a BioPAX encoded pathway. To run this function, the user needs to parse the file. It should be preceded by `readBiopax(filepath)` to obtain the biopax object. The function needs the following arguments:

- **biopax** - The BioPaX object containing the parsed data from an OWL file. This can be obtained using `readBiopax(filepath)`
- **pathwayID** - The internal ID of the pathway in the biopax object. To obtain the internal ID, the function `getPathwayID(biopax,reactomeID)` can be called

The function returns a mully graph built from the given pathway.

### *Example*

```
biopax=readBiopax(pi3k.owl)
pi3kmully=pathway2mully(biopax,"pathway1")
```

## pathwayView

### **Create an empty view**

The function is used to create a pathwayView in order to track the modifications applied to a mully graph. The object pathwayView contains different information on the View, including the timestamp of creation and last modification, the original and final version of the graph, and the dataframe containing the modification steps. The function needs the following arguments:

- **g** - The input graph
- **name** - The name of the view

The function returns an empty pathwayView Object.

### *Example*

```
view=pathwayView(mully("myMully",T),"View1")
```

## print,pathwayView

### Print Function

The function is used to print the pathwayView Object. The function needs the following arguments:

- **v** - The input pathwayView to be printed

## simplifyInteractionKegg

**Simplify the dataframe's structure** The function simplifies the interaction between a gene input and other databases and shows results in 4 columns (c1 = entry number in KEGG c2= name in other database c3= other database's name c4= organism name as attribute) The function needs the following arguments:

- **genes** - The dataframe returned by the function interactionkegg(keggInput)

### Example

```
geneList=c("hsa:122706","hsa:4221","hsa:8312")
genes = getKeggGene(geneList)
genesinteraction = interactionKegg(genes)
genesinteractionsimplified = simplifyInteractionKegg(genesinteraction)
```

## transformKeggData

**Transform data retrieved from KEGG Genes** The function translate the output of getKeggGene() into a dataframe. The function needs the following arguments:

- **list\_Get** - The list of all genes
- **list\_keggGet** - The list containing the 10 element split of list\_Get

### Example

```
geneList=c("hsa:122706","hsa:4221","hsa:8312")
genes = getKeggGene(geneList)
```

## undo

### Undo a modification step in a view

The function reverses changes applied to a mully graph, saved in a pathwayView Object. The function needs the following arguments:

- **v** - The input view
- **stps** - The number of steps to undo. This number refers to the number of unique steps' IDs to be removed, i.e. entries of steps in the view with similar stepID count as 1

The function returns The view with the undone modifications. `## wntpathway` **Demo function for Wnt Pathway Views** The function is a demo function that create a pathway mully graph from a BioPAX encoded file of the Signaling by Wnt Pathway. The function reads and parses the file, creates the mully graph, and generates 3 different views from the graph by deleting the RNA, Complex, and Physical Entity Layers. The function needs the following arguments:

- **file** - The link to the Wnt Pathway bioPAX file

***Example***

```
wntpathway(wnt_reactome.owl)
```