

Package ‘paxtoolsr’

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Type Package

Title Access Pathways from Multiple Databases Through BioPAX and Pathway Commons

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SystemRequirements Java (>= 1.6)

License LGPL-3

Description The package provides a set of R functions for interacting with BioPAX OWL files using Paxtools and the querying Pathway Commons (PC) molecular interaction database. Pathway Commons is a project by the Memorial Sloan-Kettering Cancer Center (MSKCC), Dana-Farber Cancer Institute (DFCI), and the University of Toronto. Pathway Commons databases include: BIND, BioGRID, CORUM, CTD, DIP, DrugBank, HPRD, HumanCyc, IntAct, KEGG, MirTarBase, Panther, PhosphoSitePlus, Reactome, RECON, TRANSFAC.

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<code>addAttributeList</code>	<i>Add attributes using a list of vectors to an igraph object</i>
-------------------------------	---

Description

Add attributes using a list of vectors to an igraph object

Usage

```
addAttributeList(g, attr, l)
```

Arguments

<code>g</code>	an igraph object
<code>attr</code>	the name of the attribute
<code>l</code>	the list of vectors

Value

the modified igraph object

Examples

```
library(igraph)
g <- barabasi.game(20)
g <- set_vertex_attr(g, "name", value=LETTERS[1:20])
g <- addAttributeList(g, "isProt",
  list(A=TRUE, B=FALSE, C=TRUE, D=TRUE, E=FALSE))
```

`convertDataFrameListsToVectors`*Convert columns with list in data.frame to vector*

Description

Convert columns with list in data.frame to vector

Usage

```
convertDataFrameListsToVectors(df, delimiter = ";")
```

Arguments

`df` a data.frame
`delimiter` a delimiter to concatenate (DEFAULT: ;)

Value

a data.frame without list columns

Note

Lists as columns are useful programmatically, but cause issue in writing output to text-based files

Examples

```
df <- data.frame(id = 1:2, name = c("Jon", "Mark"),  
  children = I(list(c("Mary", "James"), c("Greta", "Sally"))))  
df <- convertDataFrameListsToVectors(df)
```

`convertSifToGmt`*Convert SIF to GMT*

Description

Convert SIF to GMT

Usage

```
convertSifToGmt(sif, name = "gmt", returnSmallMolecules = FALSE)
```

Arguments

sif a data.frame representing a SIF (Simple Interaction Format)
name the name of the gene set
returnSmallMolecules a boolean whether to return genes or small molecules in the gene set

Value

a list with one entry being a vector

Examples

```
sif <- readSif(system.file("extdata", "test_sif.txt", package="paxtoolsr"))  
gmt <- convertSifToGmt(sif)
```

downloadFile	<i>Check Cache and Download File</i>
--------------	--------------------------------------

Description

Check Cache and Download File

Usage

```
downloadFile(  
  baseUrl,  
  fileName,  
  destDir = NULL,  
  cacheEnv = "PAXTOOLS_CACHE",  
  verbose = FALSE  
)
```

Arguments

baseUrl a string, entire download URL except filename
fileName a string, the filename of file to be downloaded
destDir a string, the path where a file should be saved
cacheEnv a string, environment variable pointing to specific cache
verbose show debugging information

Details

Description of file formats: <http://www.pathwaycommons.org/pc2/formats>

Value

a boolean TRUE if the file was downloaded or already exists, FALSE otherwise

See Also

[readSif](#), [readBiopax](#), [readSbgn](#), [readSifnx](#), [readGmt](#)

Examples

```
downloadFile("http://google.com/", fileName="index.html", destDir=tempdir())
```

downloadPc2

Download Pathway Commons files (uses menu and cache)

Description

Download Pathway Commons files (uses menu and cache)

Usage

```
downloadPc2(
  selectedFileName = NULL,
  destDir = NULL,
  returnNames = NULL,
  version,
  verbose = FALSE,
  ...
)
```

Arguments

selectedFileName	a string, a name of a file to skip the the interactive selection
destDir	a string, the destination directory for the file to be downloaded (Default: NULL). If NULL, then file will be downloaded to cache directory at Sys.getenv("PAXTOOLS_CACHE")
returnNames	return a vector of names matching the given regular expression
version	a version number for a previous version of Pathway Commons data; versions 3 and above. Parameter set as version="8". Available versions "http://www.pathwaycommons.org/archives/
verbose	a flag to display debugging information (Default: FALSE)
...	additional parameters to send to corresponding read* methods

Value

an R object using one of the read* methods provided in this package corresponding to the file downloaded

Examples

```
## Not run:
downloadPc2(version="8")
downloadPc2(version="8", returnNames="ext.*sif")
downloadPc2("PathwayCommons.8.inoh.GSEA.hgnc.gmt.gz", version="8", verbose=TRUE)

## End(Not run)
```

downloadSignedPC	<i>Download a SIF file containing only signed interactions</i>
------------------	--

Description

Download a SIF file containing only signed interactions

Usage

```
downloadSignedPC(destDir = NULL, forceCache = FALSE)
```

Arguments

destDir	a string, the destination directory for the file to be downloaded (Default: NULL). If NULL, then file will be downloaded to cache directory at <code>Sys.getenv("PAXTOOLS_CACHE")</code>
forceCache	a boolean to force the use of a cached version (DEFAULT: FALSE); the current host of the file (GitHub) does not support the LAST-MODIFIED header

Value

a SIF containing interactions that are considered signed (i.e. interactions causing an increase on decrease in a molecular species)

Examples

```
# downloadSignedPC()
```

fetch	<i>Fetch a set of IDs from a BioPAX OWL file</i>
-------	--

Description

This function will create a subsetting object with specified URIs.

Usage

```
fetch(inputFile, outputFile = NULL, idList)
```

Arguments

inputFile	a string of the name of the input BioPAX OWL file
outputFile	a string with the name of the output BioPAX OWL file
idList	a vector of IDs from the BioPAX OWL file

Details

Only entities in the input BioPAX file will be used in the fetch. IDs used must be URIs for the entities of interest. Additional properties such as cross-references for fetched entities will be included in the output.

Value

an XMLInternalDocument representing a BioPAX OWL file

Examples

```
outFile <- tempfile()
ids <- c("http://identifiers.org/uniprot/P36894",
        "http://identifiers.org/uniprot/Q13873")
results <- fetch(system.file("extdata", "REACT_12034-3.owl", package="paxtoolsr"),
                 outFile, ids)
```

filterSif	<i>Keep interactions in SIF network based on certain criteria</i>
-----------	---

Description

Keep interactions in SIF network based on certain criteria

Usage

```
filterSif(  
  sif,  
  ids = NULL,  
  interactionTypes = NULL,  
  dataSources = NULL,  
  interactionPubmedIds = NULL,  
  pathwayNames = NULL,  
  mediatorIds = NULL,  
  edgelist = NULL,  
  idsBothParticipants = FALSE,  
  edgelistCheckReverse = TRUE,  
  verbose = FALSE  
)
```

Arguments

sif	a binary SIF as a data.frame with three columns: "PARTICIPANT_A", "INTERACTION_TYPE", "PARTICIPANT_B"
ids	a vector of IDs to be kept
interactionTypes	a vector of interaction types to be kept (List of interaction types: http://www.pathwaycommons.org/pc2/fo)
dataSources	a vector of data sources to be kept. For Extended SIF.
interactionPubmedIds	a vector of Pubmed IDs to be kept. For Extended SIF.
pathwayNames	a vector of pathway names to be kept. For Extended SIF.
mediatorIds	a vector of mediator IDs to be kept. For Extended SIF. Mediator IDs are the full BioPAX objects that were simplified to interaction given in the SIF. For Extended SIF.
edgelist	a two-column data.frame where each row is an interaction to be kept. Directionality is ignored (e.g. Edge A B will return interactions A B and B A from SIF)
idsBothParticipants	a boolean whether both interaction participants should be in a given interaction when using the ids parameter; TRUE if both (DEFAULT: TRUE)
edgelistCheckReverse	a boolean whether to check for edges in the reverse order (DEFAULT: TRUE)
verbose	Show debugging information (DEFAULT: FALSE)

Value

filtered interactions with three columns: "PARTICIPANT_A", "INTERACTION_TYPE", "PARTICIPANT_B". The intersection of multiple filters is returned.

Examples

```
results <- readSif(system.file("extdata", "test_sif.txt", package="paxtoolsr"))
intTypes <- c("controls-state-change-of", "controls-expression-of", "catalysis-precedes")
filteredNetwork <- filterSif(results, intTypes)

tmp <- readSifnx(system.file("extdata", "test_sifnx_250.txt", package = "paxtoolsr"))
results <- filterSif(tmp$edges, ids=c("CHEBI:17640", "MCM3"))
results <- filterSif(tmp$edges, dataSources=c("INOH", "KEGG"))
results <- filterSif(tmp$edges, dataSources=c("IntAct"), ids=c("CHEBI:17640", "MCM3"))
results <- filterSif(tmp$edges, pathwayNames=c("Metabolic pathways"))
results <- filterSif(tmp$edges,
  mediatorIds=c("http://purl.org/pc2/8/MolecularInteraction_1452626895158"))
results <- filterSif(tmp$edges, interactionPubmedId="17654400")

tmp <- readSifnx(system.file("extdata", "test_sifnx_250.txt", package = "paxtoolsr"))
edgelist <- read.table(system.file("extdata", "test_edgelist.txt", package = "paxtoolsr"),
  sep="\t", header=FALSE, stringsAsFactors=FALSE)
results <- filterSif(tmp$edges, edgelist=edgelist)
```

getCacheFiles

List files in cache directory

Description

List files in cache directory

Usage

```
getCacheFiles()
```

Value

a vector of the files in the cache directory

Examples

```
getCacheFiles()
```

getErrorMessage	<i>Get Error Message for a Pathway Commons Error</i>
-----------------	--

Description

Get Error Message for a Pathway Commons Error

Usage

```
getErrorMessage(code)
```

Arguments

code	a three digit numerical error code
------	------------------------------------

Value

an error message for the code

Examples

```
results <- getErrorMessage("452")
```

getNeighbors	<i>Get the neighbors of a set of IDs in a BioPAX file</i>
--------------	---

Description

This function retrieves a set of neighbors for a set of IDs in a BioPAX file.

Usage

```
getNeighbors(inputFile, outputFile = NULL, idList)
```

Arguments

inputFile	a string with the name of the input BioPAX OWL file
outputFile	a string with the name of the output BioPAX OWL file
idList	a vector of IDs from the BioPAX OWL file

Details

Only entities in the input BioPAX file will be searched for neighbors. IDs used must be URIs for the entities of interest.

Value

an XMLInternalDocument representing a BioPAX OWL file

Examples

```
outFile <- tempfile()
results <- getNeighbors(system.file("extdata",
  "raf_map_kinase_cascade_reactome.owl", package="paxtoolsr"),
  outFile,
  c("HTTP://WWW.REACTOME.ORG/BIOPAX/48887#PROTEIN2360_1_9606",
    "HTTP://WWW.REACTOME.ORG/BIOPAX/48887#PROTEIN1631_1_9606"))
```

getPc

Get Pathway Commons BioPAX elements

Description

This command retrieves full pathway information for a set of elements such as pathway, interaction or physical entity given the RDF IDs.

Usage

```
getPc(uri, format = "BIOPAX", verbose = FALSE, ...)
```

Arguments

uri	a vector that includes valid/existing BioPAX element's URI (RDF ID; for utility classes that were "normalized", such as entity referencenes and controlled vocabularies, it is usually a Identifiers.org URL. Multiple IDs are allowed per query, for example, c("http://identifiers.org/uniprot/Q06609", "http://identifiers.org/uniprot/Q549Z0")) See also about MIRIAM and Identifiers.org in details.
format	output format (Default: BIOPAX). Valid options can be found using pcFormats
verbose	a boolean, display the command used to query Pathway Commons
...	additional arguments to read* methods that handle data from Pathway Commons

Details

Get commands only retrieve the BioPAX elements that are directly mapped to the ID. Use the "traverse query to traverse BioPAX graph and obtain child/owner elements.

Information on MIRIAM and Identifiers.org <http://www.pathwaycommons.org/pc2/#miriam>

Value

a XMLInternalDocument object

See Also

[pcFormats](#)

Examples

```
uri <- "http://identifiers.org/uniprot/014503"  
#results <- getPc(uri)  
  
uri <- c("http://identifiers.org/uniprot/014503", "http://identifiers.org/uniprot/Q9P2X7")  
#results <- getPc(uri, verbose=TRUE)
```

getPcDatabaseNames *Get a Pathway Commons Databases*

Description

Get a Pathway Commons Databases

Usage

```
getPcDatabaseNames(version)
```

Arguments

version PC2 version

Value

a names of databases that can be used as part of queries

Examples

```
getPcDatabaseNames(version=10)
```

getPcUrl	<i>Get base Pathway Commons URL</i>
----------	-------------------------------------

Description

Get base Pathway Commons URL

Usage

```
getPcUrl()
```

Details

paxtoolsr will support versions Pathway Commons 5 and later. Old versions of the webservice will not be not be operational. Users can parse older BioPAX outputs as an alternative.

Value

a string with base Pathway Commons URL

Examples

```
url <- getPcUrl()
```

getShortestPathSif	<i>Get the shortest between two IDs (HGNC or CHEBI)</i>
--------------------	---

Description

Get the shortest between two IDs (HGNC or CHEBI)

Usage

```
getShortestPathSif(  
  sif,  
  idA,  
  idB,  
  mode = c("all", "out", "in"),  
  weights = NULL,  
  verbose = FALSE,  
  filterFun,  
  ...  
)
```

Arguments

sif	a SIF network
idA	HGNC or CHEBI (CHEBI:XXXXX) ID
idB	HGNC or CHEBI (CHEBI:XXXXX) ID
mode	see <code>shortest_paths()</code> in <code>igraph</code>
weights	see <code>shortest_paths()</code> in <code>igraph</code>
verbose	a boolean whether to show debugging information
filterFun	a function to filter multiple paths of the same length
...	additional arguments passed on to <code>filterFun</code>

Value

a `data.frame` representing a SIF network

Examples

```
idA <- "DAP3"
idB <- "RPS16"
sif <- readSif(system.file("extdata", "test_sif_shortestPath.txt", package="paxtoolsr"))
filterFun <- function(vpaths) { idx <- sample(1:length(vpaths), 1); return(vpaths[[idx]]) }
m1 <- getShortestPathSif(sif, idA, idB, mode="all", weights=NULL, filterFun=filterFun, verbose=TRUE)
```

getSifInteractionCategories

Get a list of categories of SIF interactions

Description

Get a list of categories of SIF interactions

Usage

```
getSifInteractionCategories()
```

Details

Description of interaction types: <http://www.pathwaycommons.org/pc2/formats> Categories provided: `BetweenProteins`, `BetweenProteinsOther` (often from high-throughput experiments), `BetweenProteinSmallMolecule`, `BetweenSmallMolecules`, `SignedInteractions`

Value

a list of interactions in categories

Examples

```
sifCat <- getSifInteractionCategories()
sifCat[["BetweenProteins"]]
```

graphPc

*Get Pathway Commons BioPAX elements***Description**

This function will retrieve a set of BioPAX elements given a graph query match.

Usage

```
graphPc(
  kind,
  source,
  target = NULL,
  direction = NULL,
  limit = NULL,
  format = NULL,
  datasource = NULL,
  organism = NULL,
  verbose = FALSE
)
```

Arguments

kind	graph query. Valid options can be found using pcGraphQueries See Details for information on graph queries.
source	source object's URI/ID. Multiple source URIs/IDs are allowed per query, for example c("http://identifiers.org/uniprot/Q06609", "http://identifiers.org/uniprot/Q549Z0") See a note about MIRIAM and Identifiers.org in details
target	[Required for PATHSFROMTO graph query] target URI/ID. Multiple target URIs are allowed per query; for example c("http://identifiers.org/uniprot/Q06609", "http://identifiers.org/uniprot/Q549Z0") See a note about MIRIAM and Identifiers.org in details
direction	[Optional, for NEIGHBORHOOD and COMMONSTREAM algorithms] - graph search direction. Valid options: pcDirections .
limit	graph query search distance limit (default: 1).
format	output format. Valid options: pcFormats
datasource	datasource filter (same as for 'search').
organism	organism filter (same as for 'search').
verbose	a boolean, display the command used to query Pathway Commons

Value

depending on the the output format a different object may be returned. [pcFormats](#)

See Also

[pcFormats](#), [pcDirections](#)

Examples

```
source <- "http://identifiers.org/uniprot/014503"  
#results <- graphPc(source=source, kind="neighborhood", format="TXT")
```

integrateBiopax	<i>Integrate two BioPAX OWL files (DEPRECATED)</i>
-----------------	--

Description

This function merges two BioPAX OWL files

Usage

```
integrateBiopax(inputFile1, inputFile2, outputFile = NULL)
```

Arguments

inputFile1	a string of the name of the input BioPAX OWL file
inputFile2	a string of the name of the input BioPAX OWL file
outputFile	a string of the name of the output integrated BioPAX OWL file

Details

This method is deprecated. Use `mergeBiopax` instead.

Value

an XMLInternalDocument representing a BioPAX OWL file

See Also

[mergeBiopax](#)

Examples

```
outFile <- tempfile()  
results <- integrateBiopax(system.file("extdata", "raf_map_kinase_cascade_reactome.owl",  
  package="paxtoolsr"),  
  system.file("extdata", "dna_replication.owl", package="paxtoolsr"),  
  outFile)
```

loadSifInIgraph	<i>Load SIF as igraph Network</i>
-----------------	-----------------------------------

Description

Load SIF as igraph Network

Usage

```
loadSifInIgraph(sif, directed = TRUE)
```

Arguments

sif	a binary SIF as a data.frame with three columns: "PARTICIPANT_A", "INTERACTION_TYPE", "PARTICIPANT_B"
directed	a boolean weather the returned graph should be directed (DEFAULT: TRUE)

Details

Users are likely to run into issues if the input SIF has factor levels

Value

a directed igraph network with interaction types

Examples

```
results <- readSif(system.file("extdata", "test_sif.txt", package="paxtoolsr"))
g <- loadSifInIgraph(results)
```

mapAttributes	<i>Map Attributes from igraph to Cytoscape JSON</i>
---------------	---

Description

Map Attributes from igraph to Cytoscape JSON

Usage

```
mapAttributes(attr.names, all.attr, i)
```

Arguments

attr.names	names of attributes
all.attr	all attributes
i	index

Value

attributes

Note

From https://github.com/idekerlab/cy-rest-R/blob/17f748426bb5e48ba4075b9d97318ad582b250da/utility/cytoscape_util.R

mapValues

Map values from One Vector to Another

Description

Map values from One Vector to Another

Usage

```
mapValues(data, oldValue, newValue)
```

Arguments

data	a vector of strings where values will be replaced
oldValue	a vector that matches values in the data vector
newValue	a vector of new values that will replace the old values

Value

return the vector with the mapped values. If there was no corresponding entry then replace it with an NA.

Examples

```
data <- c("A", "B", "C", "X", "Y", "Z")
oldValue <- LETTERS[1:20]
newValue <- letters[1:20]
results <- mapValues(data, oldValue, newValue)
```

mergeBiopax	<i>Merges two BioPAX OWL files</i>
-------------	------------------------------------

Description

This function merges two BioPAX OWL files

Usage

```
mergeBiopax(inputFile1, inputFile2, outputFile = NULL)
```

Arguments

inputFile1	a string of the name of the input BioPAX OWL file
inputFile2	a string of the name of the input BioPAX OWL file
outputFile	a string of the name of the output merged BioPAX OWL file (Optional)

Details

Only entities that share IDs will be merged. No additional merging occurs on cross-references. Merging may result in warning messages caused as a result of redundant actions being checked against by the Java library; these messages may be ignored.

Value

an XMLInternalDocument representing a BioPAX OWL file

Examples

```
outFile <- tempfile()
results <- mergeBiopax(system.file("extdata", "raf_map_kinase_cascade_reactome.owl",
                                package="paxtoolsr"),
                      system.file("extdata", "dna_replication.owl",
                                package="paxtoolsr"),
                      outFile)
```

pcDirections

Acceptable Pathway Commons Directions

Description

A simple function to see valid options

Usage

pcDirections()

Details

- BOTHSTREAM where the current entity can either be the source or target of an interaction
- DOWNSTREAM where the current entity can only be the source
- UPSTREAM where the current entity can only be the target

Value

acceptable Pathway Commons directions

Examples

pcDirections()

pcFormats

Acceptable Pathway Commons Formats

Description

A simple function to see valid options

Usage

pcFormats()

Details

See references.

Value

acceptable Pathway Commons formats

References

Output Formats Description: <http://www.pathwaycommons.org/pc2/help/formats.html>

Examples

```
pcFormats()
```

pcGraphQueries

Acceptable Pathway Commons Graph Queries

Description

A simple function to see valid options

Usage

```
pcGraphQueries()
```

Details

- COMMONSTREAM searches common downstream or common upstream of a specified set of entities based on the given directions within the boundaries of a specified length limit
- NEIGHBORHOOD searches the neighborhood of given source set of nodes
- PATHSBETWEEN finds the paths between specific source set of states or entities within the boundaries of a specified length limit
- PATHSFROMTO finds the paths from a specific source set of states or entities to a specific target set of states or entities within the boundaries of a specified length limit

Value

acceptable Pathway Commons graph queries

Examples

```
pcGraphQueries()
```

processPcRequest	<i>Process Pathway Commons request in various formats</i>
------------------	---

Description

Process Pathway Commons request in various formats

Usage

```
processPcRequest(content, format, ...)
```

Arguments

content	a string, content to be processed
format	a string, the type of format
...	other arguments passed to read* methods for reading different formats

Value

an R object using one of the read* methods provided in this package corresponding to the format

See Also

[pcFormats](#)

Examples

```
fileName <- system.file("extdata", "test_biopax.owl", package="paxtoolsr")
content <- readChar(fileName, file.info(fileName)$size)
results <- processPcRequest(content, "BIOPAX")
```

readBiopax	<i>Read BioPAX files as XML documents</i>
------------	---

Description

Read BioPAX files as XML documents

Usage

```
readBiopax(inputFile)
```

Arguments

inputFile	an inputFile
-----------	--------------

Value

an XMLInternalDocument

Examples

```
results <- readBiopax(system.file("extdata", "biopax3-short-metabolic-pathway.owl",  
  package="paxtoolsr"))
```

readGmt

Read in gene sets from GMT files

Description

This function will read in gene sets in the GMT format into a named list.

Usage

```
readGmt(inputFile, removePrefix = FALSE, returnInfo = FALSE)
```

Arguments

inputFile	an inputFile
removePrefix	Pathway Commons genesets are prefixed with a NCBI organism taxonomy number (e.g. 9606 for humans); this is a boolean whether to remove the prefix (default: FALSE)
returnInfo	a boolean whether to return information on genesets; these results are returned a list of two items: 1) basic GMT results and 2) datasources, organism, and id type information for each gene set (default: FALSE)

Value

a named list where each entry corresponds to a gene set or a list described in the returnInfo parameter

Examples

```
f1 <- system.file("extdata", "test_PathwayCommons12.kegg.hgnc.gmt",  
  package="paxtoolsr")  
f2 <- system.file("extdata", "test_PathwayCommons12.netpath.hgnc.gmt",  
  package="paxtoolsr")  
  
results <- readGmt(f1)  
results <- readGmt(f2)  
results <- readGmt(f1, removePrefix=TRUE)  
results <- readGmt(f2, returnInfo=TRUE)
```

readPcPathwaysInfo	<i>Read in Pathway Commons Pathways Information</i>
--------------------	---

Description

Read in Pathway Commons Pathways Information

Usage

```
readPcPathwaysInfo(inputFile = NULL, version = NULL)
```

Arguments

inputFile an inputFile; if NULL then retrieve the current pathways.txt; see details (default: NULL)

version a version number for a previous version of Pathway Commons data; versions 3 and above. Parameter set as version="8". Available versions "<http://www.pathwaycommons.org/archives/>

Details

This file is generally found as pathways.txt.gz (e.g. <http://www.pathwaycommons.org/archives/PC2/current/pathways.txt.gz>)

Value

a data.frame

Examples

```
inputFile <- system.file("extdata", "pathways.txt.gz", package="paxtoolsr")
results <- readPcPathwaysInfo(inputFile, version="8")
```

readSbgn	<i>Read SBGN files as XML documents</i>
----------	---

Description

Read SBGN files as XML documents

Usage

```
readSbgn(inputFile)
```

Arguments

inputFile an inputFile

Value

an XMLInternalDocument

Examples

```
results <- readSbgn(system.file("extdata", "test_sbgn.xml", package="paxtoolsr"))
```

readSif	<i>Read in a binary SIF file</i>
---------	----------------------------------

Description

Read in a binary SIF file

Usage

```
readSif(inputFile)
```

Arguments

inputFile an inputFile

Value

a data.frame with the interactions in the binary SIF format

Examples

```
results <- readSif(system.file("extdata", "test_sif.txt", package="paxtoolsr"))
```

readSifnx	<i>Read in a Extended SIF file</i>
-----------	------------------------------------

Description

Read in a Extended SIF file

Usage

```
readSifnx(inputFile)
```

Arguments

inputFile an inputFile

Details

SIFNX files from Pathway Commons commonly come a single file that includes a tab-delimited sections for nodes and another for edges. The sections are separated by an empty lines. These sections must be split before they are read.

Value

a list with nodes and edges entries

Examples

```
results <- readSifnx(system.file("extdata", "test_sifnx.txt", package="paxtoolsr"))
```

searchListOfVectors *Search List of Vectors*

Description

Search List of Vectors

Usage

```
searchListOfVectors(q, lst)
```

Arguments

q	query vector
lst	list of vectors to search

Details

Taken from: <http://stackoverflow.com/questions/11002391/fast-way-of-getting-index-of-match-in-list>

Value

a list of vectors with the same length as the query vector, each list entry will have indices for lst where there was a match with the query vector. Return NA if there were no matches.

Examples

```
lst <- list(1:3, 3:5, 3:7)
q <- c(3, 5)
results <- searchListOfVectors(q, lst)
names(results) <- q

lst <- list(LETTERS[1:3], LETTERS[3:5], LETTERS[3:7])
q <- c("C", "E")
searchListOfVectors(q, lst)

lst <- list(LETTERS[3], LETTERS[4:6])
q <- "C"
searchListOfVectors(q, lst)

lst <- list(LETTERS[3], LETTERS[4:6])
q <- c("C")
searchListOfVectors(q, lst)

lst <- list(LETTERS[3], LETTERS[4:6])
q <- c("C", "E")
searchListOfVectors(q, lst)

lst <- list(LETTERS[3], LETTERS[4:6])
q <- "Z"
searchListOfVectors(q, lst)
```

searchPc

Search Pathway Commons

Description

This command provides a text search using the Lucene query syntax.

Usage

```
searchPc(
  q,
  page = 0,
  datasource = NULL,
  organism = NULL,
  type = NULL,
  verbose = FALSE
)
```

Arguments

q a keyword, name, external identifier, or a Lucene query string.

page	an integer giving the search result page number (N \geq 0, default: 0)
datasource	a vector that is a filter by data source (use names or URIs of pathway data sources or of any existing Provenance object). If multiple data source values are specified, a union of hits from specified sources is returned. For example, datasource as c("reactome", "pid") returns hits associated with Reactome or PID.
organism	a vector that is an organism filter. The organism can be specified either by official name, e.g. "homo sapiens" or by NCBI taxonomy id, e.g. "9606". Similar to data sources, if multiple organisms are declared a union of all hits from specified organisms is returned. For example organism as c("9606", "10016") returns results for both human and mice. Only humans, "9606" is officially supported.
type	BioPAX class filter. See Details.
verbose	a boolean, display the command used to query Pathway Commons

Details

Indexed fields were selected based on most common searches. Some of these fields are direct BioPAX properties, others are composite relationships. All index fields are (case-sensitive):comment, ecnumber, keyword, name, pathway, term, xrefdb, xrefid, dataSource, and organism. The pathway field maps to all participants of pathways that contain the keyword(s) in any of its text fields. This field is transitive in the sense that participants of all sub-pathways are also returned. Finally, keyword is a transitive aggregate field that includes all searchable keywords of that element and its child elements - e.g. a complex would be returned by a keyword search if one of its members has a match. Keyword is the default field type. All searches can also be filtered by data source and organism. It is also possible to restrict the domain class using the 'type' parameter. This query can be used standalone or to retrieve starting points for graph searches. Search strings are case insensitive unless put inside quotes.

BioPAX classes can be found at http://www.pathwaycommons.org/pc2/#biopax_types

Value

an XMLInternalDocument with results

Examples

```
query <- "Q06609"
#results <- searchPc(query)

query <- "glycolysis"
#results <- searchPc(query, type="Pathway")
```

`splitSifnxByPathway` *Splits SIFNX entries into individual pathways*

Description

Splits SIFNX entries into individual pathways

Usage

```
splitSifnxByPathway(edges, parallel = FALSE)
```

Arguments

<code>edges</code>	a data.frame with SIF content with the additional column "PATHWAY_NAMES". "PATHWAY_NAMES" should include pathway names delimited with a semi-colon: ";".
<code>parallel</code>	a boolean that will parallelize the process; requires foreach/doSNOW/parallel packages

Details

This method can be slow; ~1.5 minutes for 150K+ rows. Has a parallelized method to speed things up.

Value

a list of where each entry is a vector of row indices for a given pathway

`summarize` *Summarize a BioPAX file*

Description

This function provides a summary of BioPAX classes.

Usage

```
summarize(inputFile)
```

Arguments

<code>inputFile</code>	a string of the name of the input BioPAX OWL file
------------------------	---

Details

BioPAX classes are defined by the BioPAX specification: <http://www.biopax.org/>

Value

list with BioPAX class counts

Examples

```
summary <- summarize(system.file("extdata", "raf_map_kinase_cascade_reactome.owl",  
package="paxtoolsr"))
```

summarizeSif	<i>Summarize a SIF Network</i>
--------------	--------------------------------

Description

Summarize a SIF Network

Usage

```
summarizeSif(sif)
```

Arguments

`sif` a binary SIF as a data.frame with three columns: "PARTICIPANT_A", "INTERACTION_TYPE", "PARTICIPANT_B"

Value

a list containing a count of the unique genes in the SIF and counts for the interaction types in the network

Examples

```
results <- readSif(system.file("extdata", "test_sif.txt", package="paxtoolsr"))  
summarizeSif(results)
```

`toCytoscape`*Convert igraph to Cytoscape JSON*

Description

Convert igraph to Cytoscape JSON

Usage

```
toCytoscape(igraphobj)
```

Arguments

`igraphobj` an igraph object

Value

a JSON object

Note

From https://github.com/idekerlab/cy-rest-R/blob/17f748426bb5e48ba4075b9d97318ad582b250da/utility/cytoscape_util.R

Examples

```
library(igraph)
g <- barabasi.game(20)
json <- toCytoscape(g)
```

`toGSEA`*Converts a BioPAX OWL file to a GSEA GMT gene set*

Description

This function converts pathway information stored as BioPAX files into the the GSEA .gmt format.

Usage

```
toGSEA(  
  inputFile,  
  outputFile = NULL,  
  database = "uniprot",  
  crossSpeciesCheckFlag = TRUE  
)
```


Arguments

inputFile a string of the name of the input OWL file
outputFile a string of the name of the output file
database a string of the name of the identifier type to be included (e.g. "HGNC Symbol")
crossSpeciesCheckFlag
 a boolean that ensures participant protein is from same species

Details

The GSEA GMT format is a tab-delimited format where each row represents a gene set. The first column is the gene set name. The second column is a brief description. Other columns for each row contain genes in the gene set; these rows may be of unequal lengths.

Value

see readGmt()

Examples

```
outFile <- tempfile()
results <- toGSEA(system.file("extdata", "biopax3-short-metabolic-pathway.owl",
                             package="paxtoolsr"),
                 outFile,
                 "uniprot",
                 crossSpeciesCheckFlag=TRUE)
```

toLevel3

Convert a PSIMI or older BioPAX OWL file to BioPAX Level 3

Description

This file will convert PSIMI or older BioPAX objects to BioPAX Level 3

Usage

```
toLevel3(inputFile, outputFile = NULL)
```

Arguments

inputFile a string of the name of the input file
outputFile a string of the name of the output BioPAX OWL file

Value

an XMLInternalDocument representing a BioPAX OWL file

Examples

```
inputFile <- system.file("extdata", "raf_map_kinase_cascade_reactome.owl",
  package="paxtoolsr")
outFile <- tempfile()
results <- toLevel3(inputFile, outFile)
```

topPathways	<i>Retrieve top pathways</i>
-------------	------------------------------

Description

This command returns all "top" pathways.

Usage

```
topPathways(q = NULL, datasource = NULL, organism = NULL, verbose = FALSE)
```

Arguments

q	[Optional] a keyword, name, external identifier, or a Lucene query string, like in 'search', but the default is '*' (match all).
datasource	filter by data source (same as for 'search').
organism	organism filter (same as for 'search').
verbose	a boolean, display the command used to query Pathway Commons

Details

Pathways that are neither 'controlled' nor 'pathwayComponent' of another process.

Value

a data.frame with the following columns:

- uri URI ID for the pathway
- biopaxClass the type of BioPAX object
- name a human readable name
- dataSource the dataSource for the pathway
- organism an organism identifier
- pathway URI ID for the pathway

Examples

```
#results <- topPathways(q="TP53", datasource="panther")
```

toSBGN	<i>Convert a BioPAX OWL file to SBGNML</i>
--------	--

Description

This function will convert a BioPAX OWL file into the Systems Biology Graphical Notation (SBGN) Markup Language (SBGNML) XML representation

Usage

```
toSBGN(inputFile, outputFile = NULL)
```

Arguments

inputFile	a string of the name of the input BioPAX OWL file
outputFile	a string of the name of the output SBGNML file

Details

Objects in the SBGNML format are laid out using a Compound Spring Embedder (CoSE) layout

Value

see readSbgn()

References

<http://www.cs.bilkent.edu.tr/~ivis/layout/cose-animated-demo/cose.html>

Examples

```
outFile <- tempfile()
results <- toSBGN(system.file("extdata", "biopax3-short-metabolic-pathway.owl",
  package="paxtoolsr"),
  outFile)
```

toSif	<i>Convert a BioPAX OWL file to SIF</i>
-------	---

Description

Convert a BioPAX OWL file to a binary SIF file

Usage

```
toSif(inputFile, outputFile = NULL)
```

Arguments

inputFile	a string of the name of the input BioPAX OWL file
outputFile	a string of the name of the output SIF file (Optional)

Details

Information on SIF conversion is provided on the Pathway Commons site: <http://www.pathwaycommons.org/pc2/>

Value

see readSif()

Examples

```
outFile <- tempfile()
results <- toSif(system.file("extdata", "raf_map_kinase_cascade_reactome.owl",
  package="paxtoolsr"),
  outFile)
```

toSifnx	<i>Converts BioPAX OWL file to extended binary SIF representation</i>
---------	---

Description

Converts BioPAX OWL file to extended binary SIF representation

Usage

```
toSifnx(inputFile, outputFile = tempfile(), idType = "uniprot")
```

Arguments

inputFile	a string with the name of the input BioPAX OWL file
outputFile	a string with the name of the output file for SIFNX information
idType	a string either "hgnc" or "uniprot" (DEFAULT: uniprot, more common)

Details

Information on SIF conversion is provided on the Pathway Commons site: <http://www.pathwaycommons.org/pc2/>. Also, this is a Java-based methods, it is best to use full paths.

Value

see readSifnx()

Examples

```
inputFile <- system.file("extdata", "raf_map_kinase_cascade_reactome.owl", package="paxtoolsr")
results <- toSifnx(inputFile=inputFile)
```

traverse

Access Pathway Commons using XPath-type expressions

Description

This command provides XPath-like access to the Pathway Commons.

Usage

```
traverse(uri, path, verbose = FALSE)
```

Arguments

uri	a BioPAX element URI - specified similarly to the 'GET' command above). Multiple IDs are allowed (uri=...&uri=...&uri=...).
path	a BioPAX property path in the form of property1[:type1]/property2[:type2]; see properties, inverse properties, Paxtools, org.biopax.paxtools.controller.PathAccessor.
verbose	a boolean, display the command used to query Pathway Commons

Details

With traverse users can explicitly state the paths they would like to access. The format of the path query is in the form: [Initial Class]/[property1]:[classRestriction(optional)]/[property2]... A "*" sign after the property instructs path accessor to transitively traverse that property. For example, the following path accessor will traverse through all physical entity components within a complex: "Complex/component*/entityReference/xref:UnificationXref" The following will list display names of all participants of interactions, which are components (pathwayComponent) of a pathway (note: pathwayOrder property, where same or other interactions can be reached, is not considered here): "Pathway/pathwayComponent:Interaction/participant*/displayName" The optional parameter classRestriction allows to restrict/filter the returned property values to a certain subclass of the range of that property. In the first example above, this is used to get only the Unification Xrefs. Path accessors can use all the official BioPAX properties as well as additional derived classes and parameters in paxtools such as inverse parameters and interfaces that represent anonymous union classes in OWL. (See Paxtools documentation for more details).

Value

an XMLInternalDocument with results

References

Paxtools Documentation: <http://www.biopax.org/m2site/>

Examples

```
uri <- "http://identifiers.org/uniprot/P38398"
#results <- traverse(uri=uri, path="ProteinReference/organism/displayName")
```

validate

Validate BioPAX files

Description

This function validates BioPAX files for errors.

Usage

```
validate(
  inputFile,
  outputFile = NULL,
  type = c("xml", "html", "biopax"),
  autoFix = FALSE,
  onlyErrors = FALSE,
  maxErrors = NULL,
  notStrict = FALSE
)
```

Arguments

inputFile	a string of the name of the input BioPAX OWL file
outputFile	a string of the name of the output file containing validation results
type	a string denoting the type of output: xml (default), html, biopax
autoFix	a boolean that determines if the input file should be fixed automatically. Errors that can be automatically fixed include generating displayName properties from names, inferring organism, and inferring dataSource
onlyErrors	a boolean of whether to only display errors
maxErrors	a integer denoting the number of errors to return
notStrict	a boolean of whether to be strict in validation (default: FALSE)

Details

See the publication by Rodchenkov, et al. for information on the BioPAX validator. See <http://biopax.baderlab.org/validator> for additional information on validator. See <http://biopax.baderlab.org/validator/errorTypes.html> for information on error types.

Value

an XMLInternalDocument is returned if type is set to "xml" otherwise the location of the outputfile is returned.

References

Rodchenkov I, Demir E, Sander C, Bader GD. The BioPAX Validator, <http://www.ncbi.nlm.nih.gov/pubmed/23918249>

Examples

```
outFile <- tempfile()
rawDoc <- validate(system.file("extdata", "raf_map_kinase_cascade_reactome.owl",
  package="paxtoolsr"), onlyErrors=TRUE)
```

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