

Package ‘KEGGREST’

October 16, 2019

Version 1.24.1

Title Client-side REST access to KEGG

Author Dan Tenenbaum

Imports methods, httr, png, Biostrings

Suggests RUnit, BiocGenerics, knitr

Maintainer Bioconductor Package Maintainer

<maintainer@bioconductor.org>

Description A package that provides a client interface to the KEGG REST server. Based on KEGGSOAP by J. Zhang, R. Gentleman, and Marc Carlson, and KEGG (python package) by Aurelien Mazurie.

License Artistic-2.0

VignetteBuilder knitr

biocViews Annotation, Pathways, ThirdPartyClient, KEGG

git_url <https://git.bioconductor.org/packages/KEGGREST>

git_branch RELEASE_3_9

git_last_commit bbc3ef4

git_last_commit_date 2019-10-08

Date/Publication 2019-10-15

R topics documented:

keggConv	2
keggFind	3
keggGet	4
keggInfo	5
keggLink	6
keggList	7
listDatabases	8
mark.pathway.by.objects	9

Index	11
--------------	-----------

`keggConv`*Convert KEGG identifiers to/from outside identifiers*

Description

Convert KEGG identifiers to/from outside identifiers.

Usage

```
keggConv(target, source, querySize = 100)
```

Arguments

<code>target</code>	A KEGG organism code (), T number, or one of the external databases <code>ncbi-gi</code> , <code>ncbi-geneid</code> , <code>ncbi-proteinid</code> , <code>uniprot</code> , or (for chemical substance identifiers) <code>drug</code> , <code>compound</code> , or <code>glycan</code> , <code>pubchem</code> , or <code>chebi</code> .
<code>source</code>	Same as <code>target</code> , but may also be a list of KEGG identifiers representing internal or external names.
<code>querySize</code>	Empirically, KEGG limits queries to 100 source identifiers per query. This argument enables larger queries by dividing source into sub-queries of no more than <code>querySize</code> identifiers.

Value

A named character vector.

Author(s)

Dan Tenenbaum

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

Examples

```
## conversion from NCBI GeneID to KEGG ID for E. coli genes
head(keggConv("eco", "ncbi-geneid"))
head(keggConv("ncbi-geneid", "eco")) ## opposite direction

## conversion from KEGG ID to NCBI GI
head(keggConv("ncbi-proteinid", c("hsa:10458", "ece:Z5100")))

## conversion from NCBI GI to KEGG ID when the organism code is not known:
head(keggConv("genes", "ncbi-geneid:3113320"))
```

keggFind	<i>Finds entries with matching query keywords or other query data in a given database</i>
----------	---

Description

Finds entries with matching query keywords or other query data in a given database.

Usage

```
keggFind(database, query, option = c("formula", "exact_mass",  
  "mol_weight"))
```

Arguments

database	Either the name of a single KEGG database (list available via <code>listDatabases()</code> , a "T number" genome identifier, or a KEGG organism code (lists of both available via <code>keggList("organism")</code>).
query	One or more keywords, or a range of integers representing molecular weights. If query includes identifiers not known to KEGG, the results will not contain any information about those identifiers.
option	Optional. If database is compound or drug, option can be formula, exact_mass, or weight. Chemical formula search is a partial match irrespective of the order of atoms given. The exact mass (or molecular weight) is checked by rounding off to the same decimal place as the query data.

Value

A named character vector.

Author(s)

Dan Tenenbaum

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

Examples

```
res <-  
  keggFind("genes", c("shiga", "toxin")) ## for keywords "shiga" and "toxin"  
length(res)  
head(res)  
res <- keggFind("genes", "shiga toxin")  ## for keywords "shiga toxin"  
length(res)  
head(res)  
keggFind("compound", "C7H10O5", "formula") ## for chemical formula "C7H10O5"  
res <- keggFind("compound", "O5C7", "formula") ## for chemical formula  
  ## containing "O5" and "C7"  
  
length(res)  
head(res)
```

```
keggFind("compound", 174.05, "exact_mass") ## for 174.045
                                     ## =< exact mass < 174.055
res <- keggFind("compound", 300:310, "mol_weight") ## for 300 =<
                                     ## molecular weight =< 310

length(res)
head(res)
```

keggGet

Retrieves given database entries

Description

Retrieves given database entries.

Usage

```
keggGet(dbentries, option = c("aaseq", "ntseq", "mol", "kcf",
                              "image", "kgml"))
```

Arguments

dbentries	One or more (up to a maximum of 10) KEGG identifiers.
option	Optional. Option governing the format of the output. aaseq is an amino acid sequence, ntseq is a nucleotide sequence. image returns an object which can be written to a PNG file, kgml returns a KGML document.

Details

Retrieves all entries from the KEGG database for a set of KEGG identifiers.

keggGet() can only return 10 result sets at once (this limitation is on the server side). If you supply more than 10 inputs to keggGet(), KEGGREST will warn that only the first 10 results will be returned.

Value

A list wrapping a KEGG flat file. If option is aaseq, an AAStringSet object. If option is ntseq, a DNASTringSet object. If option is image, an object which can be written to a PNG file. If option is kgml, a KGML document.

Author(s)

Dan Tenenbaum

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

Examples

```
res <- keggGet(c("cpd:C01290", "gl:G00092")) ## retrieves a compound entry
                                         ## and a glycan entry
str(res)
res <- keggGet(c("C01290", "G00092")) ## same as above, without prefixes
str(res)
res <- keggGet(c("hsa:10458", "ece:Z5100")) ## retrieves a human gene entry
                                         ## and an E.coli 0157 gene entry
str(res)
res <- keggGet(c("hsa:10458", "ece:Z5100"), "aaseq") ## retrieves amino
                                         ## acid sequences of a human gene and an
                                         ## E.coli 0157 gene
png <- keggGet("hsa05130", "image") ## retrieves the image file of a
                                         ## pathway map

t <- tempfile()
library(png)
writePNG(png, t)
res <- keggGet("hsa05130", "kgml")
str(res)
```

keggInfo

Displays the current statistics of a given database

Description

Displays statistics of a given database, such as number of entries, version, release date, and source.

Usage

```
keggInfo(database)
```

Arguments

database	Either a KEGG database (list available via listDatabases()), a KEGG organism code (list available by calling keggList() with the organism argument), or a T number (list available by calling keggList() with the genome argument.)
----------	--

Value

A character vector containing statistics about database.

Author(s)

Dan Tenenbaum

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

Examples

```
res <- keggInfo("kegg") ## displays the current statistics of the KEGG database
cat(res)
res <- keggInfo("pathway") ## displays the number pathway entries including both
                           ## the reference and organism-specific pathways
cat(res)
res <- keggInfo("hsa") ## displays the number of gene entries for the
                       ## KEGG organism Homo sapiens
cat(res)
```

keggLink

Find related entries by using database cross-references.

Description

Find related entries by using database cross-references.

Usage

```
keggLink(target, source)
```

Arguments

target	Either the name of a single KEGG database (list available via <code>listDatabases()</code> , a "T number" genome identifier, or a KEGG organism code (lists of both available via <code>keggList("organism")</code>).
source	The same as target, but may also be one or more KEGG identifiers.

Details

Many of the old KEGGSOAP functions whose names started with 'get', such as `get.pathways.by.genes` and `get.pathways.by.reactions`, are replaced by using `keggLink` (see examples).

Value

A named character vector.

Author(s)

Dan Tenenbaum

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

Examples

```
res <- keggLink("pathway", "hsa") ## KEGG pathways linked from each of
      ## the human genes equivalent to 'get.genes.by.pathway' in KEGGSOAP
length(res)
head(res)
res <- keggLink("hsa", "pathway") ## human genes linked from each of the
      ## KEGG pathways equivalent to 'get.pathways.by.genes' in KEGGSOAP
keggLink("pathway", c("hsa:10458", "ece:Z5100")) ## KEGG pathways
      ## linked from a human gene and an E. coli 0157 gene
res <- keggLink("hsa:126") ## LinkDB search shows all KEGG
      ## resources related to hsa:126
head(res)
```

keggList

Returns a list of entry identifiers and associated definition for a given database or a given set of database entries.

Description

Returns a list of entry identifiers and associated definition for a given database or a given set of database entries.

Usage

```
keggList(database, organism)
```

Arguments

database	Either a KEGG database (list available via listDatabases()), a KEGG organism code (list available via keggList() with the organism argument), a T number (list available via keggList() with the genome argument), or a character vector of KEGG identifiers.
organism	Optional. A KEGG organism identifier (list available via keggList() with the organism argument).

Value

A named character vector containing entry identifiers and associated definition.

Author(s)

Dan Tenenbaum

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

Examples

```
res <- keggList("pathway") ## returns the list of reference pathways
length(res)
head(res)
res <- keggList("pathway", "hsa") ## returns the list of human pathways
length(res)
head(res)
res <- keggList("organism") ## returns the list of KEGG organisms with
                           ## taxonomic classification

nrow(res)
head(res)
res <- keggList("hsa") ## returns the entire list of human genes
length(res)
head(res)
## keggList("T01001") ## same as above
keggList(c("hsa:10458", "ece:Z5100")) ## returns the list of a human gene
                                     ## and an E.coli 0157 gene
keggList(c("cpd:C01290", "gl:G00092")) ## returns the list of a compound entry
                                     ## and a glycan entry
keggList(c("C01290+G00092")) ## same as above (prefixes are not necessary)
```

listDatabases

Lists the KEGG databases which may be searched.

Description

Lists the KEGG databases which may be searched. In most cases, you can also use a KEGG organism name or T number (genome identifier) as a database name.

Usage

```
listDatabases()
```

Value

A character vector of database names.

Author(s)

Dan Tenenbaum

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

See Also

[keggList](#)

Examples

```
listDatabases()
res <- keggList("organism") ## list all organisms
nrow(res)
head(res)
res <- keggList("hsa") ## list all human genes
length(res)
head(res)
## keggList("T01001") ## list all human genes
res <- keggList("genome") ## list all genome identifiers
length(res)
head(res)
```

```
mark.pathway.by.objects
```

Client-side interface to obtain an url for a KEGG pathway diagram with a given set of genes marked

Description

Given a KEGG pathway id and a set of KEGG gene ids, the functions return the URL of a KEGG pathway diagram with the elements corresponding to the genes marked by red or specified color

Usage

```
mark.pathway.by.objects(pathway.id, object.id.list)
color.pathway.by.objects(pathway.id, object.id.list,
                          fg.color.list, bg.color.list)
```

Arguments

pathway.id	pathway.id a character string for a KEGG pathway id. KEGG pathway ids consist of the string path followed by a colon, a three-letter code for the organism of concern, and then a number (e. g. "path:eco00020"). The three-letter organism code consists of the first letter of the genus name and the first two letters of the species name of the scientific name of the organism of concern
object.id.list	object.id.list a vector of character strings for KEGG gene ids. KEGG gene ids normally consist of three letters followed by a column and then several numeric numbers. The three letters are from the first letter of the genus name and the first two letters of the species name of the scientific name of the organism of concern (e. g. hsa:111 for Homo Sapiens)
fg.color.list	fg.color.list a vector of two character strings to indicate the color for the text and border, respectively, of the objects in a pathway diagram. The strings can either be a color code like <code>\#ff0000</code> or letter like yellow
bg.color.list	bg.color.list a vector of character strings of the same length of object.id.list to indicate the background color of the objects in a pathway diagram. The strings can either be a color code like <code>\#ff0000</code> or letter like yellow

Details

This function only returns the URL of the KEGG pathway diagram. Use the function [browseURL](#) to view the diagram.

These functions are not part of the KEGG REST API; they are provided because they existed in KEGGSOAP and an alternative implementation was possible.

Value

This function returns a character string for the url

Author(s)

Jianhua Zhang

References

<https://www.kegg.jp/kegg/docs/keggapi.html>

See Also

[browseURL](#)

Examples

```
url <- mark.pathway.by.objects(
  "path:eco00260", c("eco:b0002", "eco:c00263")
)
if(interactive()){
  browseURL(url)
}
url <- color.pathway.by.objects(
  "path:eco00260", c("eco:b0002", "eco:c00263"),
  c("#ff0000", "#00ff00"),
  c("#ffff00", "yellow")
)
```

Index

- *Topic **conv**
 - keggConv, 2
- *Topic **databases**
 - listDatabases, 8
- *Topic **database**
 - listDatabases, 8
- *Topic **datasets**
 - mark.pathway.by.objects, 9
- *Topic **find**
 - keggFind, 3
- *Topic **get**
 - keggGet, 4
- *Topic **info**
 - keggInfo, 5
- *Topic **link**
 - keggLink, 6
- *Topic **list**
 - keggList, 7
- *Topic **metadata**
 - keggInfo, 5

bconv (keggConv), 2
browseURL, 10

color.pathway.by.objects
 (mark.pathway.by.objects), 9
conv (keggConv), 2

info (keggInfo), 5

keggConv, 2
keggFind, 3
keggGet, 4
keggInfo, 5
keggLink, 6
keggList, 5, 7, 7, 8

link (keggLink), 6
listDatabases, 3, 5–7, 8

mark.pathway.by.objects, 9