Package ‘KEGGREST’

May 29, 2024

Version  1.44.0
Title    Client-side REST access to the Kyoto Encyclopedia of Genes and Genomes (KEGG)
Depends  R (>= 3.5.0)
Imports  methods, httr, png, Biostrings
Suggests RUnit, BiocGenerics, knitr, markdown
Description A package that provides a client interface to the Kyoto Encyclopedia of Genes and Genomes (KEGG) REST API. Only for academic use by academic users belonging to academic institutions (see <https://www.kegg.jp/kegg/rest/>).
Note that KEGGREST is based on KEGGSOAP by J. Zhang, R. Gentleman, and Marc Carlson, and KEGG (python package) by Aurelien Mazurie.
URL       https://bioconductor.org/packages/KEGGREST
BugReports https://github.com/Bioconductor/KEGGREST/issues
License   Artistic-2.0
VignetteBuilder knitr
biocViews Annotation, Pathways, ThirdPartyClient, KEGG
RoxygenNote 7.1.1
git_url    https://git.bioconductor.org/packages/KEGGREST
git_branch RELEASE_3_19
git_last_commit 6d110a0
git_last_commit_date 2024-04-30
Repository Bioconductor 3.19
Date/Publication 2024-05-29
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keggCompounds

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keggCompounds  Get list of compounds IDs for pathway

Description
Get list of compounds IDs for pathway.

Usage
keggCompounds(pathwayID)

Arguments
  pathwayID  A KEGG pathway identifier with the prefix map and 5 digit number.

Value
A list of KEGG compound identifiers

Author(s)
Dan Tenenbaum, Kristina Riemer

References
  https://www.genome.jp/kegg/pathway.html

Examples
  keggCompounds("map00361")
keggConv

Convert KEGG identifiers to/from outside identifiers

Description

Convert KEGG identifiers to/from outside identifiers.

Usage

keggConv(target, source, querySize = 100)

Arguments

target  A KEGG organism code (), T number, or one of the external databases ncbi-gi, ncbi-geneid, ncbi-proteinid, uniprot, or (for chemical substance identifiers) drug, compound, or glycan, pubchem, or chebi.

source  Same as target, but may also be a list of KEGG identifiers representing internal or external names.

querySize  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 querySize 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  

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

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 listDatabases()), a "T number" genome identifier, or a KEGG organism code (lists of both available via keggList("organism")).

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

```r
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 DNADStringSet 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

```r
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 O157 gene entry
str(res)
res <- keggGet(c("hsa:10458", "ece:Z5100"), "aaseq") ## retrieves amino
## acid sequences of a human gene and an
## E.coli O157 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)
```

display the current statistics of a given database

Displays the current 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

```r
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

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

Arguments

- `target`  
  Either the name of a single KEGG database (list available via `listDatabases()`), a "T number" genome identifier, or a KEGG organism code (lists of both available via `keggList("organism")`).

- `source`  
  The same as `target`, but may also be one or more KEGG identifiers.

Details

Many of the old KEGG SOAP 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

```r
res <- keggLink("pathway", "hsa") ## KEGG pathways linked from each of
## the human genes equivalent to 'get.genes.by.pathway' in KEGG SOAP
length(res)
head(res)
res <- keggLink("hsa", "pathway") ## human genes linked from each of the
## KEGG pathways equivalent to 'get.pathways.by.genes' in KEGG SOAP
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](https://www.kegg.jp/kegg/docs/keggapi.html)
**Examples**

```r
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**

```r
listDatabases()
```

**Value**

A character vector of database names.

**Author(s)**

Dan Tenenbaum

**References**

[https://www.kegg.jp/kegg/docs/keggapi.html](https://www.kegg.jp/kegg/docs/keggapi.html)

**See Also**

keggList
Examples

```r
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

```r
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` : 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` : 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` : 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 #ff0000 or letter like yellow

- `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 #ff0000 or letter like yellow
**mark.pathway.by.objects**

**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**

```r
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("#ff0000", "yellow")
)```
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