

Package ‘pathview’

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Type Package

Title a tool set for pathway based data integration and visualization

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Description Pathview is a tool set for pathway based data integration and visualization. It maps and renders a wide variety of biological data on relevant pathway graphs. All users need is to supply their data and specify the target pathway. Pathview automatically downloads the pathway graph data, parses the data file, maps user data to the pathway, and render pathway graph with the mapped data. In addition, Pathview also seamlessly integrates with pathway and gene set (enrichment) analysis tools for large-scale and fully automated analysis.

biocViews Pathways, GraphAndNetwork, Visualization, GeneSetEnrichment, DifferentialExpression, GeneExpression, Microarray, RNASeq, Genetics, Metabolomics, Proteomics, SystemsBiology, Sequencing

Depends R (>= 2.10), KEGGgraph, org.Hs.eg.db

Imports Rgraphviz, graph, png, AnnotationDbi, KEGGREST, methods, utils

Suggests gage, org.Mm.eg.db, RUnit, BiocGenerics

License GPL (>=3.0)

URL <http://pathview.r-forge.r-project.org/>

LazyLoad yes

R topics documented:

pathview-package	2
combineKEGGnodes	3
cpd.accs	4
cpdidmap	5
demo.data	6
download.kegg	7
eg2id	8
kegg.species.code	10
korg	11
mol.sum	12
node.color	13
node.info	16
node.map	17
pathview	19
sim.mol.data	26
wordwrap	28

Index	30
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pathview-package	<i>Pathway based data integration and visualization</i>
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Description

Pathway based data integration and visualization

Details

Package:	pathview
Type:	Package
Version:	1.0
Date:	2012-12-26
License:	What license is it under?
LazyLoad:	yes

~~ An overview of how to use the package, including the most important ~~ functions ~~

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

combineKEGGnodes *Special treatment of nodes or edges for KEGG pathway rendering*

Description

combineKEGGnodes combines nodes into a group in a KEGG pathway graph. reaction2edge converts reactions into edges in KEGG pathway graph.

Usage

```
combineKEGGnodes(nodes, graph, combo.node)
reaction2edge(path, gR)
```

Arguments

nodes	character, names of the names to be combined.
graph, gR	a object of "graphNEL" class, the graph parsed and converted from KEGG pathway.
path	a object of "KEGGPathway" class, the parsed KEGG pathway.
combo.node	character, the name of result combined node.

Details

combineKEGGnodes not only combines nodes in the graph object, but also corresponding node data in the KEGG pathway object. This function is needed for KEGG-defined group nodes and parsed enzyme groups involved in the same reaction. reaction2edge converts a reaction into 2 consecutive edges between substrate and enzyme and enzyme and product. This function is needed as to faithfully show the compound-enzyme nodes and their interactions in Graphviz-style view of KEGG pathway.

Value

The results returned by combineKEGGnodes is a combined graph of "graphNEL" class. The results returned by reaction2edge is a list of 3 elements: gR, the converted graph ("graphNEL"); edata.new, the new edge data ("KEGGEdge"); ndata.new, the new node data ("KEGGNode").

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[node.info](#) the main parser function

cpd.accs

Mapping data between compound or gene IDs and KEGG accessions

Description

Mapping data between compound or gene IDs and KEGG accessions

Usage

```
data(cpd.accs)
data(cpd.names)
data(kegg.met)
data(ko.ids)
data(rn.list)
data(gene.idtype.list)
data(cpd.simtypes)
```

Format

cpd.accs is a data frame with 30054 observations on the following 4 variables. cpd.names is a data frame with 12314 observations on the following 5 variables. kegg.met is a character matrix of 694 rows and 3 columns. ko.ids is a character vector 8511 KEGG ortholog gene IDs, as used in KEGG ortholog pathways. rn.list is a namedlist of 21 vectors. Each vector records the row numbers for one of 21 different compound ID types in cpd.accs data.frame. gene.idtype.list is a character vector of 10 common gene, transcript or protein ID types. cpd.simtypes is a character vector of 7 common compound related ID types, each of them has over 1000 unique entries. Hence these ID types are good for generating simulation compound data.

Source

ftp://ftp.ebi.ac.uk/pub/databases/chebi/Flat_file_tab_delimited/

http://www.genome.jp/kegg-bin/get_htext?br08001.keg

Examples

```

data(cpd.accs)
data(rn.list)
names(rn.list)
cpd.accs[rn.list[[1]][1:4],]
lapply(rn.list[1:4], function(rn) cpd.accs[rn[1:4],])

data(kegg.met)
head(kegg.met)

```

cpdidmap

*Mapping between compound IDs and KEGG accessions***Description**

These auxillary compound ID mappers connect KEGG compound/glycan/drug accessions to compound names/synonyms and other commonly used compound-related IDs.

Usage

```

cpdidmap(in.ids, in.type, out.type)
cpd2kegg(in.ids, in.type)
cpdkegg2name(in.ids, in.type = c("KEGG", "KEGG COMPOUND accession")[1])
cpdname2kegg(in.ids)

```

Arguments

<code>in.ids</code>	character, input IDs to be mapped.
<code>in.type</code>	character, the input ID type, needs to be either "KEGG" (including compound, glycan and durg) or one of the compound-related ID types used in ChEMBL database. For a full list of the ChEMBL IDs, do <code>data(rn.list)</code> ; <code>names(rn.list)</code> . For <code>cpdkegg2name</code> , default <code>in.type = "KEGG"</code> .
<code>out.type</code>	character, the output ID type, needs to be either "KEGG" (including compound/glycan/durg) or one of the compound-related ID types used in ChEMBL database. For a full list of the ChEMBL IDs, do <code>data(rn.list)</code> ; <code>names(rn.list)</code> .

Details

character, the output ID type, needs to be either "KEGG" or one of the compound-related ID types used in ChEMBL database. For a full list of the ChEMBL IDs, do `data(rn.list)`; `names(rn.list)`.

KEGG has its own compound ID system, including compound (glycan/durg) accessions. Therefore, all compound data need to be mapped to KEGG accessions when working with KEGG pathways. Function `cpd2kegg` does this mapping by calling `cpdname2kegg` or `cpdidmap`. On the other hand, we frequently want to check or show compound full names or other commonly used IDs instead of the less informative KEGG accessions when working with KEGG compound nodes, Functions `cpdkegg2name` and `cpdidmap` do this reverse mapping. These functions are written as part of the

Pathview mapper module, they are equally useful for other compound ID or data mapping tasks. The use of these functions depends on a few data objects: "cpd.accs", "cpd.names", "keg.met" and "rn.list", which are included in this package. To access them, use `data()` function.

Value

a 2-column character matrix recording the mapping between input IDs to the target ID type.

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[eg2id](#) and [id2eg](#) the auxillary gene ID mappers, [mol.sum](#) the auxillary molecular data mapper, [node.map](#) the node data mapper function.

Examples

```
data(cpd.simtypes)
#generate simulated compound data named with non-KEGG ("CAS Registry Number")IDs
cpd.cas <- sim.mol.data(mol.type = "cpd", id.type = cpd.simtypes[2],
  nmol = 10000)
#construct map between non-KEGG ID and KEGG ID ("KEGG COMPOUND accession")
id.map.cas <- cpdidmap(in.ids = names(cpd.cas), in.type = cpd.simtypes[2],
  out.type = "KEGG COMPOUND accession")
#Map molecular data onto standard KEGG IDs
cpd.kc <- mol.sum(mol.data = cpd.cas, id.map = id.map.cas)
#check the results
head(cpd.cas)
head(id.map.cas)
head(cpd.kc)

#map KEGG ID to compound name
cpd.names=cpdkegg2name(in.ids=id.map.cas[,2])
head(cpd.names)
```

Description

demo.paths includes pathway ids and optimal plotting parameters when calling pathway.

GSE16873 is a breast cancer study (Emery et al, 2009) downloaded from Gene Expression Omnibus (GEO). Dataset gse16873 is pre-processed using FARMS method and includes 6 patient cases, each with HN (histologically normal) and DCIS (ductal carcinoma in situ) RMA samples. The same dataset is also used in gage package. Dataset gse16873.d includes the gene expression changes of two pairs of DCIS vs HN samples.

Usage

```
data(demo.paths)
data(gse16873.d)
```

Format

demo.paths is a named list with ids and plotting parameters for 3 pathways. For details do:

```
data(demo.paths); demo.paths
```

gse16873.d is a numeric matrix with over 10000 rows (genes) and 2 columns (samples). For details do: data(gse16873.d); str(gse16873.d).

Source

<http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE16873>

download.kegg

Download KEGG pathway graphs and associated KGML data

Description

This is the downloader function for KEGG pathways, automatically download graph images and associated KGML data.

Usage

```
download.kegg(pathway.id = "00010", species = "hsa", kegg.dir = ".")
```

Arguments

pathway.id	character, 5-digit KEGG pathway IDs. Default pathway.id="00010".
species	character, either the KEGG code, scientific name or the common name of the target species. When KEGG ortholog pathway is considered, species="ko". Default species="hsa", it is equivalent to use either "Homo sapiens" (scientific name) or "human" (common name).
kegg.dir	character, the directory of KEGG pathway data file (.xml) and image file (.png). Default kegg.dir="." (current working directory).

Details

Species can be specified as either kegg code, scientific name or the common name. Scientific name and the common name are always mapped to kegg code first. Length of species should be either 1 or the same as pathway.id, if not, the same set of pathway.id will be applied to all species.

Value

a named character vector, either "succeed" or "failed", indicating the download status of corresponding pathways.

Author(s)

Weijun Luo <luo_weijun@yahoo.com>

References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[pathview](#) the main function, [node.info](#) the parser,

Examples

```
data(demo.paths)
sel.2paths=demo.paths$sel.paths[1:2]
download.kegg(pathway.id = sel.2paths, species = "hsa")
#pathway files should be downloaded into current working directory
```

eg2id

Mapping between Entrez Gene and other IDs

Description

These auxillary gene ID mappers connect Entrez Gene ID to external gene, transcript or protein IDs or vise versa.

Usage

```
eg2id(eg, category = gene.idtype.list[1:2], org = "Hs", pkg.name = NULL)
id2eg(ids, category = gene.idtype.list[1], org = "Hs", pkg.name = NULL)
```


Arguments

eg	character, input Entrez Gene IDs.
ids	character, input gene/transcript/protein IDs to be converted to Entrez Gene IDs.
category	character, for eg2id the output ID types to map from Entrez Gene, d to be c("SYMBOL", "GENENAME"); for id2eg, the input ID type to be mapped to Entrez Gene, default to be "SYMBOL".
org	character, the two-letter abbreviation of organism name, used to determine the gene annotation package. Default org="Hs". Only effective when pkg.name is not NULL.
pkg.name	character, name of the gene annotation package. This package should be one of the standard annotation packages from Bioconductor, such as "org.Hs.eg.db". Check data(bods); bods for a full list of standard annotation packages. You may also use your custom annotation package built with AnnotationDbi, the Bioconductor Annotation Database Interface. Default pkg.name=NULL, hence argument org should be specified.

Details

KEGG uses Entrez Gene ID as its standard gene ID. Therefore, all gene data need to be mapped to Entrez Genes when working with KEGG pathways. Function `id2eg` does this mapping. On the other hand, we frequently want to check or show gene symbols or full names instead of the less informative Entrez Gene ID when working with KEGG gene nodes, Function `eg2id` does this reverse mapping. These functions are written as part of the Pathview mapper module, they are equally useful for other gene ID or data mapping tasks. The use of these functions depends on gene annotation packages like "org.Hs.eg.db", which are Bioconductor standard. If no such packages are available for your interesting organisms, you may build one with Bioconductor AnnotationDbi package.

Value

a 2- or multi-column character matrix recording the mapping between input IDs to the target ID type(s).

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[cpd2kegg](#) etc the auxiliary compound ID mappers, [mol.sum](#) the auxiliary molecular data mapper, [node.map](#) the node data mapper function.

Examples

```

data(gene.idtype.list)
#generate simulated gene data named with non-KEGG/Entrez gene IDs
gene.ensprot <- sim.mol.data(mol.type = "gene", id.type = gene.idtype.list[4],
  nmol = 50000)
#construct map between non-KEGG ID and KEGG ID (Entrez gene)
id.map.ensprot <- id2eg(ids = names(gene.ensprot),
  category = gene.idtype.list[4], org = "Hs")
#Map molecular data onto Entrez Gene IDs
gene.entrez <- mol.sum(mol.data = gene.ensprot, id.map = id.map.ensprot)
#check the results
head(gene.ensprot)
head(id.map.ensprot)
head(gene.entrez)

#map Entrez Gene to Gene Symbol and Name
eg.symbname=eg2id(eg=id.map.ensprot[,2])
#entries with more than 1 Entrez Genes are not mapped
head(eg.symbname)

```

kegg.species.code *Mapping species name to KEGG code*

Description

This function maps species name to KEGG code.

Usage

```
kegg.species.code(species = "hsa", na.rm = FALSE, code.only = TRUE)
```

Arguments

species	character, either the KEGG code, scientific name or the common name of the target species. Default species="hsa", it is equivalent to use either "Homo sapiens" (scientific name) or "human" (common name).
na.rm	logical, should unmapped entris be removed. Default na.rm = FALSE.
code.only	logical, whether to extract KEGG species code only or with gene ID usage info too. Default , code.only = TRUE.

Value

a character vector of mapped KEGG code of species.

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[korg](#) the species and KEGG code mapping data, [cpd2kegg](#) etc the auxillary compound ID mappers, [download.kegg](#) the downloader function.

Examples

```
species=c("ptr", "Mus musculus", "dog", "happ")
kcode=kegg.species.code(species = species, na.rm = FALSE)
print(kcode)
```

korg	<i>Mapping data on KEGG species code and corresponding Bioconductor gene annotation package</i>
------	---

Description

Data on KEGG species, including KEGG code, scientific name, common name, corresponding gene ID types, and gene annotation package names in Bioconductor

Usage

```
data(korg)
data(bods)
```

Format

korg is a character matrix of ~3000 rows and 6 columns. First 3 columns are KEGG species code, scientific name and common name, followed columns on gene ID types used for each species: entrez.gnodes ("1" or "0", whether EntrezGene is the default gene ID) and representative KEGG gene ID and EntrezGene ID.

bods is a character matrix of 19 rows and 3 columns on the mapping between gene annotation package names in Bioconductor, common name and KEGG code of most common research species.

Source

```
http://www.genome.jp/kegg-bin/get_htext?br08601.keg
http://bioconductor.org/packages/release/BiocViews.html#___OrgDb
```

Examples

```
data(korg)
data(bods)
head(korg)
head(bods)
```

mol.sum

*Mapping and summation of molecular data onto standard IDs***Description**

Molecular data like gene or metabolite data are frequently annotated by various types of IDs. This function maps and summarize molecular data onto standard gene or compound IDs. It would be straightforward to integrate, analyze or visualize the "standardized" data with pathways or functional categories.

Usage

```
mol.sum(mol.data, id.map, gene.annotpkg = "org.Hs.eg.db", sum.method =
c("sum", "mean", "median", "max", "max.abs", "random")[1])
```

Arguments

mol.data	Either vector (single sample) or a matrix-like data (multiple sample). Vector should be numeric with molecule IDs as names or it may also be character of molecule IDs. Character vector is treated as discrete or count data. Matrix-like data structure has molecules as rows and samples as columns. Row names should be molecule IDs. Default mol.data=NULL. This argument is equivalent to gene.data or cpd.data in the pathview function. Check pathview function for more information.
id.map	a two-column character matrix, giving the mapping between molecular IDs used in mol.data and target/standard molecular IDs. Then mol.data are gene data, id.map may also be a character specifying the type of IDs used in mol.data. The two-column mapping matrix will be generated automatically.
gene.annotpkg	character, name of the gene annotation package. This package should be one of the standard annotation packages from Bioconductor, such as "org.Hs.eg.db" (default). Check data(bods); bods for a full list of standard annotation packages. You may also use your custom annotation package built with AnnotationDbi, the Bioconductor Annotation Database Interface. Only effective when mol.data are gene.data and id.map gives the ID type being used.
sum.method	character, the method name to calculate node summary given that multiple genes or compounds are mapped to it. Potential options include "sum", "mean", "median", "max", "max.abs" and "random". Default sum.method="sum".

Details

This function is called in pathview main function when gene.idtype or cpd.idtype is not the standard type, so that the molecular data can be mapped and summarized onto standard IDs. This is needed for further mapping to KEGG pathways. The same standard ID mapping is needed when carry out pathway or functional analysis on molecular data, which are labeled by non-standard (or alien) IDs or probe names, like in most of the microarray or metabolomics datasets. In other words, function mol.sum can be useful in all these situations.

Value

a numeric vector or matrix. Its dimensionality is the same as the input mol.data except row names are standard molecular IDs.

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[node.map](#) the node data mapper function. [id2eg](#), [cpd2kegg](#) etc the auxillary molecular ID mappers, [pathview](#) the main function,

Examples

```
data(gene.idtype.list)
#generate simulated gene data named with non-KEGG/Entrez gene IDs
gene.ensprot <- sim.mol.data(mol.type = "gene", id.type = gene.idtype.list[4],
  nmol = 50000)
#construct map between non-KEGG ID and KEGG ID (Entrez gene)
id.map.ensprot <- id2eg(ids = names(gene.ensprot),
  category = gene.idtype.list[4], org = "Hs")
#Map molecular data onto Entrez Gene IDs
gene.entrez <- mol.sum(mol.data = gene.ensprot, id.map = id.map.ensprot)
#check the results
head(gene.ensprot)
head(id.map.ensprot)
head(gene.entrez)
```

node.color

Code molecular data as pseudo colors on the pathway graph

Description

node.color converts the mapped molecular (gene, protein or metabolite etc) data as pseudo colors on pathway nodes. col.key draws color key(s) for mapped molecular data on the pathway graph.

Usage

```
node.color(plot.data = NULL, discrete=FALSE, limit, bins, both.dirs =
TRUE, low = "green", mid = "gray", high = "red", na.col = "transparent",
trans.fun = NULL)
col.key(discrete=FALSE, limit = 1, bins = 10, cols = NULL, both.dirs =
TRUE, low = "green", mid = "gray", high = "red", graph.size, node.size,
size.by.graph = TRUE, key.pos = "topright", off.sets = c(x = 0, y = 0),
align = "n", cex = 1, lwd = 1)
```

Arguments

plot.data	the result returned by node.map function. It is a data.frame composed of parsed KGML data and summary molecular data for each mapped node. Rows are mapped nodes, and columns are parsed or mapped node data. Check node.map for details.
discrete	logical, whether to treat the molecular data or node summary data as discrete. d discrete=FALSE, otherwise, mol.data will be a character vector of molecular IDs.
limit	a list of two numeric elements with "gene" and "cpd" as the names. This argument specifies the limit values for gene.data and cpd.data when converting them to pseudo colors. Each element of the list could be of length 1 or 2. Length 1 suggests discrete data or 1 directional (positive-valued) data, or the absolute limit for 2 directional data. Length 2 suggests 2 directional data. Default limit=list(gene=0.5, cpd=1).
bins	a list of two integer elements with "gene" and "cpd" as the names. This argument specifies the number of levels or bins for gene.data and cpd.data when converting them to pseudo colors. Default limit=list(gene=10, cpd=10).
both.dirs	a list of two logical elements with "gene" and "cpd" as the names. This argument specifies whether gene.data and cpd.data are 1 directional or 2 directional data when converting them to pseudo colors. Default limit=list(gene=TRUE, cpd=TRUE).
trans.fun	a list of two function (not character) elements with "gene" and "cpd" as the names. This argument specifies whether and how gene.data and cpd.data are transformed. Examples are log, abs or users' own functions. Default limit=list(gene=NULL, cpd=NULL).
low, mid, high	each is a list of two colors with "gene" and "cpd" as the names. This argument specifies the color spectra to code gene.data and cpd.data. When data are 1 directional (TRUE value in both.dirs), only mid and high are used to specify the color spectra. Default spectra (low-mid-high) "green"- "gray"- "red" and "blue"- "gray"- "yellow" are used for gene.data and cpd.data respectively. The values for 'low, mid, high' can be given as color names ('red'), plot color index (2=red), and HTML-style RGB, ("#FF0000"=red).
na.col	color used for NA's or missing values in gene.data and cpd.data. d na.col="transparent".
cols	character, specifying a discrete spectrum of colors to be plotted as color key. Note this argument is usually NULL (default), otherwise, the number of discrete colors has to match bins.

<code>graph.size</code>	numeric vector of length 2, i.e. the sizes (width, height) of the pathway graph panel. This is needed to determine the sizes and exact location of the color key.
<code>node.size</code>	numeric vector of length 2, i.e. the sizes (width, height) of the standard gene nodes (rectangles). This is needed to determine the sizes and exact location of the color key when <code>size.by.graph=FALSE</code> .
<code>size.by.graph</code>	logical, whether to determine the sizes and exact location of the color key with respect to the size of the whole graph panel or that of a single node. Default <code>size.by.graph=TRUE</code> .
<code>key.pos</code>	character, controlling the position of color key(s). Potential values are "bottom-left", "bottomright", "topleft" and "topright". Default <code>key.pos="topright"</code> .
<code>off.sets</code>	numeric vector of length 2, with "x" and "y" as the names. This argument specifies the offset values in x and y axes when plotting a new color key, as to avoid overlap with existing color keys or boundaries. Note that the <code>off.sets</code> value is reset and returned each time <code>col.key</code> function is called, as for the reference of plotting the next color key. Default <code>off.sets=c(0,0)</code> .
<code>align</code>	character, controlling how the color keys are aligned when needed. Potential values are "x", aligned by x coordinates, and "y", aligned by y coordinates. Default <code>align="x"</code> .
<code>cex</code>	A numerical value giving the amount by which legend text and symbols should be scaled relative to the default 1.
<code>lwd</code>	numeric, the line width, a <code>_positive_</code> number, defaulting to '1'.

Details

`node.color` converts the mapped molecular data (`gene.data` or `cpd.data`) by `node.map` function into pseudo colors, which then can be plotted on the pathway graph. `col.key` is used in combination with `node.color` in `pathview`, although this function can be used independently for similar tasks.

Value

`node.color` returns a vector or matrix of colors. Its dimensionality is the same as the corresponding `gene.data` or `cpd.data`. `col.key` plots a color key on existing pathway graph, then returns an updated version of `off.sets` for the reference of next color key.

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[keggview.native](#) and [keggview.graph](#) the viewer functions, [node.map](#) the node data mapper function.

Examples

```
xml.file=system.file("extdata", "hsa04110.xml", package = "pathview")
node.data=node.info(xml.file)
names(node.data)
data(gse16873.d)
plot.data.gene=node.map(mol.data=gse16873.d[,1], node.data,
  node.types="gene")
head(plot.data.gene)
cols.ts.gene=node.color(plot.data.gene, limit=1, bins=10)
head(cols.ts.gene)
```

node.info

Extract node information from KEGG pathway

Description

The parser function, parser KGML file and/or extract node information from KEGG pathway.

Usage

```
node.info(object, short.name = TRUE)
```

Arguments

object	either a character specifying the full KGML file name (with directory), or a object of "KEGGPathway" class, or a object of "graphNEL" class. The latter two are parsed results of KGML file.
short.name	logical, if TRUE, the short labels, i.e. the first item separated by "," in the long labels are parsed out as node labels. Default short.name=TRUE.

Details

Parser function node.info extract node data from parsed KEGG pathways. KGML files are parsed using parseKGML2 and KEGGpathway2Graph2. These functions from KEGGgraph package have been heavily modified for reaction parsing and conversion to edges.

Value

a named list of 10 elements: "kegg.names", "type", "component", "size", "labels", "shape", "x", "y", "width" and "height". Each elements record the corresponding attribute for all nodes in the parsed KEGG pathway.

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[pathview](#) the main function, [combineKEGGnodes](#) and [reaction2edge](#) for special treatment of nodes or edges.

Examples

```
xml.file=system.file("extdata", "hsa04110.xml", package = "pathview")
node.data=node.info(xml.file)
names(node.data)
#or parse into a graph object, then extract node info
gR1=pathview::parseKGM2Graph2(xml.file, genesOnly=FALSE, expand=FALSE, split.group=FALSE)
node.data=node.info(gR1)
```

node.map

Map molecular data onto KEGG pathway nodes

Description

The mapper function, mapping molecular data(gene expression, metabolite abundance etc)to nodes in KEGG pathway.

Usage

```
node.map(mol.data = NULL, node.data, node.types = c("gene", "ortholog",
"compound")[1], node.sum = c("sum", "mean", "median", "max", "max.abs",
"random")[1], entrez.gnodes=TRUE)
```

Arguments

mol.data	Either vector (single sample) or a matrix-like data (multiple sample). Vector should be numeric with molecule IDs as names or it may also be character of molecule IDs. Character vector is treated as discrete or count data. Matrix-like data structure has molecules as rows and samples as columns. Row names should be molecule IDs. Default mol.data=NULL. This argument is equivalent to gene.data or cpd.data in the pathview function. Check pathview function for more information.
node.data	a named list of 10 elements, the results returned by node.info, check the function for details.
node.types	character, specify the node type to map the mol.data to, either "gene", "compound", or "ortholog". Default node.types="gene".

node.sum	character, the method name to calculate node summary given that multiple genes or compounds are mapped to it. Potential options include "sum", "mean", "median", "max", "max.abs" and "random". Default node.sum="sum".
entrez.gnodes	logical, whether EntrezGene (NCBI GeneID) is used as the default gene ID in the KEGG data files. This is needed because KEGG uses different types default gene ID for different species. Some most common model species use EntrezGene, but majority of others use Locus tag. Default entrez.gnodes=TRUE.

Details

Mapper function node.map maps user supplied molecular data to KEGG pathways. This function takes standard KEGG molecular IDs (Entrez Gene ID or KEGG Compound Accession) and map them to pathway nodes. None KEGG molecular gene IDs or Compound IDs are pre-mapped to standard KEGG IDs by calling another function mol.sum. When multiple molecules map to one node, the corresponding molecular data are summarized into a single node summary by calling function specified by node.sum. This mapped node summary data together with the parsed KGML data are then returned for further processing. Proper input data include: gene expression, protein expression, genetic association, metabolite abundance, genomic data, literature, and other data types mappable to pathways. The input mol.data may be NULL, then no molecular data are actually mapped, but all nodes of the specified node.type are considered "mappable" and their parsed KGML data returned.

Value

A data.frame composed of parsed KGML data and summary molecular data for each mapped node. Each row is a mapped node, and columns are:

kegg.names	standard KEGG IDs/Names for mapped nodes. It's Entrez Gene ID or KEGG Compound Accessions.
labels	Node labels to be used when needed
type	node type, currently 4 types are supported: "gene", "enzyme", "compound" and "ortholog".
x	x coordinate in the original KEGG pathway graph.
y	y coordinate in the original KEGG pathway graph.
width	node width in the original KEGG pathway graph.
height	node height in the original KEGG pathway graph.
other columns	columns of the mapped gene/compound data

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

`mol.sum` the auxiliary molecular data mapper, `id2eg`, `cpd2kegg` etc the auxiliary molecular ID mappers, `node.color` the node color coder, `pathview` the main function, `node.info` the parser.

Examples

```
xml.file=system.file("extdata", "hsa04110.xml", package = "pathview")
node.data=node.info(xml.file)
names(node.data)
data(gse16873.d)
plot.data.gene=node.map(mol.data=gse16873.d[,1], node.data,
  node.types="gene")
head(plot.data.gene)
```

 pathview

Pathway based data integration and visualization

Description

Pathview is a tool set for pathway based data integration and visualization. It maps and renders user data on relevant pathway graphs. All users need is to supply their gene or compound data and specify the target pathway. Pathview automatically downloads the pathway graph data, parses the data file, maps user data to the pathway, and render pathway graph with the mapped data. Pathview generates both native KEGG view and Graphviz views for pathways. `keggview.native` and `keggview.graph` are the two viewer functions, and `pathview` is the main function providing a unified interface to downloader, parser, mapper and viewer functions.

Usage

```
pathview(gene.data = NULL, cpd.data = NULL, xml.file = NULL, pathway.id,
  species = "hsa", kegg.dir = ".", cpd.idtype = "kegg", gene.idtype =
  "entrez", gene.annotpkg = NULL, min.nnodes = 3, kegg.native = TRUE,
  map.null = TRUE, expand.node = FALSE, split.group = FALSE, map.symbol =
  TRUE, map.cpdname = TRUE, node.sum = "sum", discrete=list(gene=FALSE,
  cpd=FALSE), limit = list(gene = 1, cpd = 1), bins = list(gene = 10, cpd
  = 10), both.dirs = list(gene = T, cpd = T), trans.fun = list(gene =
  NULL, cpd = NULL), low = list(gene = "green", cpd = "blue"), mid =
  list(gene = "gray", cpd = "gray"), high = list(gene = "red", cpd =
  "yellow"), na.col = "transparent", ...)
```

```
keggview.native(plot.data.gene = NULL, plot.data.cpd = NULL,
  cols.ts.gene = NULL, cols.ts.cpd = NULL, node.data, pathway.name,
  out.suffix = "pathview", kegg.dir = ".", multi.state=TRUE, match.data =
  TRUE, same.layer = TRUE, res = 300, cex = 0.25, discrete =
  list(gene=FALSE, cpd=FALSE), limit= list(gene = 1, cpd = 1), bins =
  list(gene = 10, cpd = 10), both.dirs =list(gene = T, cpd = T), low =
  list(gene = "green", cpd = "blue"), mid = list(gene = "gray", cpd =
```

```
"gray"), high = list(gene = "red", cpd = "yellow"), na.col =
"transparent", new.signature = TRUE, plot.col.key = TRUE, key.align =
"x", key.pos = "topright", ...)
```

```
keggview.graph(plot.data.gene = NULL, plot.data.cpd = NULL, cols.ts.gene
= NULL, cols.ts.cpd = NULL, node.data, path.graph, pathway.name,
out.suffix = "pathview", pdf.size = c(7, 7), multi.state=TRUE,
same.layer = TRUE, match.data = TRUE, rankdir = c("LR", "TB")[1],
is.signal = TRUE, split.group = F, afactor = 1, text.width = 15, cex =
0.5, map.cpdname = FALSE, cpd.lab.offset = 1.0,
discrete=list(gene=FALSE, cpd=FALSE), limit = list(gene = 1, cpd = 1),
bins = list(gene = 10, cpd = 10), both.dirs = list(gene = T, cpd = T),
low = list(gene = "green", cpd = "blue"), mid = list(gene = "gray", cpd
= "gray"), high = list(gene = "red", cpd = "yellow"), na.col =
"transparent", new.signature = TRUE, plot.col.key = TRUE, key.align =
"x", key.pos = "topright", sign.pos = "bottomright", ...)
```

Arguments

gene.data	either vector (single sample) or a matrix-like data (multiple sample). Vector should be numeric with gene IDs as names or it may also be character of gene IDs. Character vector is treated as discrete or count data. Matrix-like data structure has genes as rows and samples as columns. Row names should be gene IDs. Here gene ID is a generic concepts, including multiple types of gene, transcript and protein uniquely mappable to KEGG gene IDs. KEGG ortholog IDs are also treated as gene IDs as to handle metagenomic data. Check details for mappable ID types. Default gene.data=NULL. numeric, character, continuous
cpd.data	the same as gene.data, except named with IDs mappable to KEGG compound IDs. Over 20 types of IDs included in ChEMBL database can be used here. Check details for mappable ID types. Default cpd.data=NULL. Note that gene.data and cpd.data can't be NULL simultaneously.
xml.file	character, the KGML data file name without directory path. Directory path is supplied with kegg.dir argument.
pathway.id	character, the KEGG pathway ID, usually 5 digit, may also include the 3 letter KEGG species code.
species	character, either the kegg code, scientific name or the common name of the target species. This applies to both pathway and gene.data or cpd.data. When KEGG ortholog pathway is considered, species="ko". Default species="hsa", it is equivalent to use either "Homo sapiens" (scientific name) or "human" (common name).
kegg.dir	character, the directory of KEGG pathway data file (.xml) and image file (.png). Default kegg.dir="." (current working directory).
cpd.idtype	character, ID type used for the cpd.data. Default cpd.idtype="kegg" (include compound, glycan and drug accessions).
gene.idtype	character, ID type used for the gene.data, case insensitive. Default gene.idtype="entrez", i.e. Entrez Gene, which are the primary KEGG gene ID for many common

model organisms. For other species, `gene.idtype` should be set to "KEGG" as KEGG use other types of gene IDs. For the common model organisms (to check the list, do: `data(bods); bods`), you may also specify other types of valid IDs. To check the ID list, do: `data(gene.idtype.list); gene.idtype.list`.

<code>gene.annotpkg</code>	character, the name of the annotation package to use for mapping between other gene ID types including symbols and Entrez gene ID. Default <code>gene.annotpkg=NULL</code> .
<code>min.nnodes</code>	integer, minimal number of nodes of type "gene", "enzyme", "compound" or "ortholog" for a pathway to be considered. Default <code>min.nnodes=3</code> .
<code>kegg.native</code>	logical, whether to render pathway graph as native KEGG graph (.png) or using graphviz layout engine (.pdf). Default <code>kegg.native=TRUE</code> .
<code>map.null</code>	logical, whether to map the NULL <code>gene.data</code> or <code>cpd.data</code> to pathway. When NULL data are mapped, the gene or compound nodes in the pathway will be rendered as actually mapped nodes, except with NA-valued color. When NULL data are not mapped, the nodes are rendered as unmapped nodes. This argument mainly affects native KEGG graph view, i.e. when <code>kegg.native=TRUE</code> . Default <code>map.null=TRUE</code> .
<code>expand.node</code>	logical, whether the multiple-gene nodes are expanded into single-gene nodes. Each expanded single-gene nodes inherits all edges from the original multiple-gene node. This option only affects graphviz graph view, i.e. when <code>kegg.native=FALSE</code> . This option is not effective for most metabolic pathways where it conflicts with converting reactions to edges. Default <code>expand.node=FALSE</code> .
<code>split.group</code>	logical, whether split node groups are split to individual nodes. Each split member nodes inherits all edges from the node group. This option only affects graphviz graph view, i.e. when <code>kegg.native=FALSE</code> . This option also effects most metabolic pathways even without group nodes defined originally. For these pathways, genes involved in the same reaction are grouped automatically when converting reactions to edges unless <code>split.group=TRUE</code> . Default <code>split.group=FALSE</code> .
<code>map.symbol</code>	logical, whether map gene IDs to symbols for gene node labels or use the graphic name from the KGML file. This option is only effective for <code>kegg.native=FALSE</code> or <code>same.layer=FALSE</code> when <code>kegg.native=TRUE</code> . For <code>same.layer=TRUE</code> when <code>kegg.native=TRUE</code> , the native KEGG labels will be kept. Default <code>map.symbol=TRUE</code> .
<code>map.cpdname</code>	logical, whether map compound IDs to formal names for compound node labels or use the graphic name from the KGML file (KEGG compound accessions). This option is only effective for <code>kegg.native=FALSE</code> . When <code>kegg.native=TRUE</code> , the native KEGG labels will be kept. Default <code>map.cpdname=TRUE</code> .
<code>node.sum</code>	character, the method name to calculate node summary given that multiple genes or compounds are mapped to it. Potential options include "sum", "mean", "median", "max", "max.abs" and "random". Default <code>node.sum="sum"</code> .
<code>discrete</code>	a list of two logical elements with "gene" and "cpd" as the names. This argument tells whether <code>gene.data</code> or <code>cpd.data</code> should be treated as discrete. Default <code>discrete=list(gene=FALSE, cpd=FALSE)</code> , i.e. both data should be treated as continuous.
<code>limit</code>	a list of two numeric elements with "gene" and "cpd" as the names. This argument specifies the limit values for <code>gene.data</code> and <code>cpd.data</code> when converting them to pseudo colors. Each element of the list could be of length 1 or 2.

	Length 1 suggests discrete data or 1 directional (positive-valued) data, or the absolute limit for 2 directional data. Length 2 suggests 2 directional data. Default <code>limit=list(gene=0.5, cpd=1)</code> .
<code>bins</code>	a list of two integer elements with "gene" and "cpd" as the names. This argument specifies the number of levels or bins for <code>gene.data</code> and <code>cpd.data</code> when converting them to pseudo colors. Default <code>limit=list(gene=10, cpd=10)</code> .
<code>both.dirs</code>	a list of two logical elements with "gene" and "cpd" as the names. This argument specifies whether <code>gene.data</code> and <code>cpd.data</code> are 1 directional or 2 directional data when converting them to pseudo colors. Default <code>limit=list(gene=TRUE, cpd=TRUE)</code> .
<code>trans.fun</code>	a list of two function (not character) elements with "gene" and "cpd" as the names. This argument specifies whether and how <code>gene.data</code> and <code>cpd.data</code> are transformed. Examples are <code>log</code> , <code>abs</code> or users' own functions. Default <code>limit=list(gene=NULL, cpd=NULL)</code> .
<code>low, mid, high</code>	each is a list of two colors with "gene" and "cpd" as the names. This argument specifies the color spectra to code <code>gene.data</code> and <code>cpd.data</code> . When data are 1 directional (TRUE value in <code>both.dirs</code>), only <code>mid</code> and <code>high</code> are used to specify the color spectra. Default spectra (low-mid-high) "green"- <code>"gray"</code> - <code>"red"</code> and <code>"blue"</code> - <code>"gray"</code> - <code>"yellow"</code> are used for <code>gene.data</code> and <code>cpd.data</code> respectively. The values for 'low, mid, high' can be given as color names (<code>'red'</code>), plot color index (<code>2=red</code>), and HTML-style RGB, (<code>"\#FF0000"=red</code>).
<code>na.col</code>	color used for NA's or missing values in <code>gene.data</code> and <code>cpd.data</code> . d <code>na.col="transparent"</code> .
<code>...</code>	extra arguments passed to <code>keggview.native</code> or <code>keggview.graph</code> function. special arguments for <code>keggview.native</code> or <code>keggview.graph</code> function.
<code>plot.data.gene</code>	<code>data.frame</code> returned by <code>node.map</code> function for rendering mapped gene nodes, including node name, type, positions (x, y), sizes (width, height), and mapped <code>gene.data</code> . This data is also used as input for pseudo-color coding through <code>node.color</code> function. Default <code>plot.data.gene=NULL</code> .
<code>plot.data.cpd</code>	same as <code>plot.data.gene</code> function, except for mapped compound node data. d <code>plot.data.cpd=NULL</code> . Default <code>plot.data.cpd=NULL</code> . Note that <code>plot.data.gene</code> and <code>plot.data.cpd</code> can't be NULL simultaneously.
<code>cols.ts.gene</code>	vector or matrix of colors returned by <code>node.color</code> function for rendering <code>gene.data</code> . Dimensionality is the same as the latter. Default <code>cols.ts.gene=NULL</code> .
<code>cols.ts.cpd</code>	same as <code>cols.ts.gene</code> , except corresponding to <code>cpd.data</code> . d <code>cols.ts.cpd=NULL</code> . Note that <code>cols.ts.gene</code> and <code>cols.ts.cpd</code> <code>plot.data.gene</code> can't be NULL simultaneously.
<code>node.data</code>	list returned by <code>node.info</code> function, which parse KGML file directly or indirectly, and extract the node data.
<code>pathway.name</code>	character, the full KEGG pathway name in the format of 3-letter species code with 5-digit pathway id, eg "hsa04612".
<code>out.suffix</code>	character, the suffix to be added after the pathway name as part of the output graph file. Sample names or column names of the <code>gene.data</code> or <code>cpd.data</code> are also added when there are multiple samples. Default <code>out.suffix="pathview"</code> .

multi.state	logical, whether multiple states (samples or columns) gene.data or cpd.data should be integrated and plotted in the same graph. Default match.data=TRUE. In other words, gene or compound nodes will be sliced into multiple pieces corresponding to the number of states in the data.
match.data	logical, whether the samples of gene.data and cpd.data are paired. Default match.data=TRUE. When let sample sizes of gene.data and cpd.data be m and n, when m>n, extra columns of NA's (mapped to no color) will be added to cpd.data as to make the sample size the same. This will result in the same number of slice in gene nodes and compound when multi.state=TRUE.
same.layer	logical, control plotting layers: 1) if node colors be plotted in the same layer as the pathway graph when kegg.native=TRUE, 2) if edge/node type legend be plotted in the same page when kegg.native=FALSE.
res	The nominal resolution in ppi which will be recorded in the bitmap file, if a positive integer. Also used for 'units' other than the default, and to convert points to pixels. This argument is only effective when kegg.native=TRUE. Default res=300.
cex	A numerical value giving the amount by which plotting text and symbols should be scaled relative to the default 1. Default cex=0.25 when kegg.native=TRUE, cex=0.5 when kegg.native=FALSE.
new.signature	logical, whether pathview signature is added to the pathway graphs. Default new.signature=TRUE.
plot.col.key	logical, whether color key is added to the pathway graphs. Default plot.col.key=TRUE.
key.align	character, controlling how the color keys are aligned when both gene.data and cpd.data are not NULL. Potential values are "x", aligned by x coordinates, and "y", aligned by y coordinates. Default key.align="x".
key.pos	character, controlling the position of color key(s). Potential values are "bottomleft", "bottomright", "topleft" and "topright". Default key.pos="topright".
sign.pos	character, controlling the position of pathview signature. Only effective when kegg.native=FALSE, Signature position is fixed in place of the original KEGG signature when kegg.native=TRUE. Potential values are "bottomleft", "bottomright", "topleft" and "topright". Default sign.pos="bottomright".
path.graph	a graph object parsed from KGML file, only effective when kegg.native=FALSE.
pdf.size	a numeric vector of length 2, giving the width and height of the pathway graph pdf file. Note that pdf width increase by half when same.layer=TRUE to accommodate legends. Only effective when kegg.native=FALSE. Default pdf.size=c(7,7).
rankdir	character, either "LR" (left to right) or "TB" (top to bottom), specifying the pathway graph layout direction. Only effective when kegg.native=FALSE. Default rank.dir="LR".
is.signal	logical, if the pathway is treated as a signaling pathway, where all the unconnected nodes are dropped. This argument also affect the graph layout type, i.e. "dot" for signals or "neato" otherwise. Only effective when kegg.native=FALSE. Default is.signal=TRUE.

<code>afactor</code>	numeric, node amplifying factor. This argument is for node size fine-tuning, its effect is subtler than expected. Only effective when <code>kegg.native=FALSE</code> . Default <code>afactor=1</code> .
<code>text.width</code>	numeric, specifying the line width for text wrap. Only effective when <code>kegg.native=FALSE</code> . Default <code>text.width=15</code> (characters).
<code>cpd.lab.offset</code>	numeric, specifying how much compound labels should be put above the default position or node center. This argument is useful when <code>map.cpdname=TRUE</code> , i.e. compounds are labelled by full name, which affects the look of compound nodes and color. Only effective when <code>kegg.native=FALSE</code> . Default <code>cpd.lab.offset=1.0</code> .

Details

Pathview maps and renders user data on relevant pathway graphs. Pathview is a stand alone program for pathway based data integration and visualization. It also seamlessly integrates with pathway and functional analysis tools for large-scale and fully automated analysis. Pathview provides strong support for data Integration. It works with: 1) essentially all types of biological data mappable to pathways, 2) over 10 types of gene or protein IDs, and 20 types of compound or metabolite IDs, 3) pathways for over 2000 species as well as KEGG orthology, 4) various data attributes and formats, i.e. continuous/discrete data, matrices/vectors, single/multiple samples etc. To see mappable external gene/protein IDs do: `data(gene.idtype.list)`, to see mappable external compound related IDs do: `data(rn.list); names(rn.list)`. Pathview generates both native KEGG view and Graphviz views for pathways. Currently only KEGG pathways are implemented. Hopefully, pathways from Reactome, NCI and other databases will be supported in the future.

Value

The result returned by `pathview` function is a named list, with 2 elements ("`plot.data.gene`", "`plot.data.cpd`"). Both elements are `data.frame` or `NULL` depends on the corresponding input data `gene.data` and `cpd.data`. These `data.frames` record the plot data for mapped gene or compound nodes: rows are mapped genes/compounds, columns are:

<code>kegg.names</code>	standard KEGG IDs/Names for mapped nodes. It's Entrez Gene ID or KEGG Compound Accessions.
<code>labels</code>	Node labels to be used when needed
<code>type</code>	node type, currently 4 types are supported: "gene", "enzyme", "compound" and "ortholog".
<code>x</code>	x coordinate in the original KEGG pathway graph.
<code>y</code>	y coordinate in the original KEGG pathway graph.
<code>width</code>	node width in the original KEGG pathway graph.
<code>height</code>	node height in the original KEGG pathway graph.
<code>other columns</code>	columns of the mapped gene/compound data and corresponding pseudo-color codes for individual samples

The results returned by `keggview.native` and `codekeggview.graph` are both a list of graph plotting parameters. These are not intended to be used externally.

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[download.kegg](#) the downloader, [node.info](#) the parser, [node.map](#) and [node.color](#) the mapper.

Examples

```
#load data
data(gse16873.d)
data(demo.paths)

#KEGG view: gene data only
i <- 1
pv.out <- pathview(gene.data = gse16873.d[, 1], pathway.id =
demo.paths$sel.paths[i], species = "hsa", out.suffix = "gse16873",
kegg.native = TRUE)
str(pv.out)
head(pv.out$plot.data.gene)
#result PNG file in current directory

#Graphviz view: gene data only
pv.out <- pathview(gene.data = gse16873.d[, 1], pathway.id =
demo.paths$sel.paths[i], species = "hsa", out.suffix = "gse16873",
kegg.native = FALSE, sign.pos = demo.paths$spos[i])
#result PDF file in current directory

#KEGG view: both gene and compound data
sim.cpd.data=sim.mol.data(mol.type="cpd", nmol=3000)
i <- 3
print(demo.paths$sel.paths[i])
pv.out <- pathview(gene.data = gse16873.d[, 1], cpd.data = sim.cpd.data,
pathway.id = demo.paths$sel.paths[i], species = "hsa", out.suffix =
"gse16873.cpd", keys.align = "y", kegg.native = TRUE, key.pos = demo.paths$npos1[i])
str(pv.out)
head(pv.out$plot.data.cpd)

#multiple states in one graph
set.seed(10)
sim.cpd.data2 = matrix(sample(sim.cpd.data, 18000,
replace = TRUE), ncol = 6)
pv.out <- pathview(gene.data = gse16873.d[, 1:3],
cpd.data = sim.cpd.data2[, 1:2], pathway.id = demo.paths$sel.paths[i],
species = "hsa", out.suffix = "gse16873.cpd.3-2s", keys.align = "y",
kegg.native = TRUE, match.data = FALSE, multi.state = TRUE, same.layer = TRUE)
str(pv.out)
```

```

head(pv.out$plot.data.cpd)

#result PNG file in current directory

##more examples of pathview usages are shown in the vignette.

```

sim.mol.data

Simulate molecular data for pathview experiment

Description

The molecular data simulator generates either gene.data or cpd.data of different ID types, molecule numbers, sample sizes, either continuous or discrete.

Usage

```

sim.mol.data(mol.type = c("gene", "gene.ko", "cpd")[1], id.type = NULL,
species="hsa", discrete = FALSE, nmol = 1000, nexp = 1, rand.seed=100)

```

Arguments

mol.type	character of length 1, specifying the molecular type, either "gene" (including transcripts, proteins), or "gene.ko" (KEGG ortholog genes, as defined in KEGG ortholog pathways), or "cpd" (including metabolites, glycans, drugs). Note that KEGG ortholog gene are considered "gene" in function pathview. Default mol.type="gene".
id.type	character of length 1, the molecular ID type. When mol.type="gene", proper ID types include "KEGG" and "ENTREZ" (Entrez Gene). Other ID types are also valid When species="hsa" only, check: data(gene.idtype.list); gene.idtype.list for other valid ID types. When mol.type="cpd", check data(cpd.simtypes); cpd.simtypes for valid ID types. Default id.type=NULL, then "Entrez" and "KEGG COMPOUND accession" will be assumed for mol.type = "gene" or "cpd".
species	character, either the kegg code, scientific name or the common name of the target species. This is only effective when mol.type = "gene". Setting species="ko" is equivalent to mol.type="gene.ko". Default species="hsa", equivalent to either "Homo sapiens" (scientific name) or "human" (common name), gene data id.type has multiple other choices. When other species are specified, gene id.type is limited to "KEGG" and "ENTREZ".
discrete	logical, whether to generate discrete or continuous data. d discrete=FALSE, otherwise, mol.data will be a character vector of molecular IDs.
nmol	integer, the target number of different molecules. Note that the specified id.type may not have as many different IDs as nmol. In this case, all IDs of id.type are used.
nexp	integer, the sample size or the number of columns in the result simulated data.
rand.seed	numeric of length 1, the seed number to start the random sampling process. This argumemnt makes the simulation reproducible as long as its value keeps the same. Default rand.seed=100.

Details

This function is written mainly for simulation or experiment with pathview package. With the simulated molecular data, you may check whether and how pathview works for molecular data of different types, IDs, format or sample sizes etc. You may also generate both gene.data and cpd.data and check data pathway based integration with pathview.

Value

either vector (single sample) or a matrix-like data (multiple sample), depends on the value of nexp. Vector should be numeric with molecular IDs as names or it may also be character of molecular IDs depending on the value of discrete. Matrix-like data structure has molecules as rows and samples as columns. Row names should be molecular IDs.

This returned data can be used directly as gene.data or cpd.data input of pathview main function.

Author(s)

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References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

[node.map](#) the node data mapper function. [mol.sum](#) the auxillary molecular data mapper, [id2eg](#), [cpd2kegg](#) etc the auxillary molecular ID mappers, [pathview](#) the main function,

Examples

```
#continuous compound data
cpd.data.c=sim.mol.data(mol.type="cpd", nmol=3000)
#discrete compound data
cpd.data.d=sim.mol.data(mol.type="cpd", nmol=3000, discrete=TRUE)
head(cpd.data.c)
head(cpd.data.d)
#continuous compound data named with "CAS Registry Number"
cpd.cas <- sim.mol.data(mol.type = "cpd", id.type = "CAS Registry Number", nmol = 10000)

#gene data with two samples
gene.data.2=sim.mol.data(mol.type="gene", nmol=1000, nexp=2)
head(gene.data.2)

#KEGG ortholog gene data
ko.data=sim.mol.data(mol.type="gene.ko", nmol=5000)
```

`wordwrap`*Wrap or break strings into lines of specified width*

Description

`strfit` does hard wrapping, i.e. break within long words, `wordwrap` is a wrapper of `strfit` but also provides soft wrapping option, i.e. break only between words, and keep long words intact.

Usage

```
wordwrap(s, width = 20, break.word = FALSE)
strfit(s, width = 20)
```

Arguments

<code>s</code>	character, strings to be wrapped or broken down.
<code>width</code>	integer, target line width in terms of number of characters. default width=20.
<code>break.word</code>	logical, whether to break within words or only between words as to fit the line width. Default <code>break.word=FALSE</code> , i.e. keep words intact and only break between words. Therefore, some line may exceed the width limit.

Details

These functions are called as to wrap long node labels into shorter lines on pathway graphs in `keggview.graph` function (when `keggview.native=FALSE`). They are equally useful for wrapping long labels in other types of graphs or output formats.

Value

character of the same length of `s` except that each element has been wrapped softly or hardly.

Author(s)

Weijun Luo <luo_weijun@yahoo.com>

References

Luo, W. and Brouwer, C., Pathview: an R/Bioconductor package for pathway based data integration and visualization. *Bioinformatics*, 2013, 29(14): 1830-1831, doi: 10.1093/bioinformatics/btt285

See Also

`strwrap` in R base.

Examples

```
long.str="(S)-Methylmalonate semialdehyde"  
wr1=wordwrap(long.str, width=15)  
#long word intact  
cat(wr1, sep="\n")  
wr2=strfit(long.str, width=15)  
#long word split  
cat(wr2, sep="\n")
```

Index

*Topic **\textasciitildekwd1**

- combineKEGGnodes, 3
- cpdidmap, 5
- download.kegg, 7
- eg2id, 8
- kegg.species.code, 10
- mol.sum, 12
- node.color, 13
- node.info, 16
- node.map, 17
- pathview, 19
- sim.mol.data, 26
- wordwrap, 28

*Topic **\textasciitildekwd2**

- combineKEGGnodes, 3
- cpdidmap, 5
- download.kegg, 7
- eg2id, 8
- kegg.species.code, 10
- mol.sum, 12
- node.color, 13
- node.info, 16
- node.map, 17
- pathview, 19
- sim.mol.data, 26
- wordwrap, 28

*Topic **datasets**

- cpd.accs, 4
- demo.data, 6
- korg, 11

*Topic **package**

- pathview-package, 2

bods (korg), 11

- col.key (node.color), 13
- combineKEGGnodes, 3, 17
- cpd.accs, 4
- cpd.names (cpd.accs), 4
- cpd.simtypes (cpd.accs), 4

- cpd2kegg, 9, 11, 13, 19, 27
- cpd2kegg (cpdidmap), 5
- cpdidmap, 5
- cpdkegg2name (cpdidmap), 5
- cpdname2kegg (cpdidmap), 5

- demo.data, 6
- demo.paths (demo.data), 6
- download.kegg, 7, 11, 25

eg2id, 6, 8

- gene.idtype.list (cpd.accs), 4
- gse16873.d (demo.data), 6

id2eg, 6, 13, 19, 27

id2eg (eg2id), 8

- kegg.met (cpd.accs), 4
- kegg.species.code, 10
- keggview.graph, 15
- keggview.graph (pathview), 19
- keggview.native, 15
- keggview.native (pathview), 19
- ko.ids (cpd.accs), 4
- korg, 11, 11

mol.sum, 6, 9, 12, 19, 27

- node.color, 13, 19, 25
- node.info, 4, 8, 16, 19, 25
- node.map, 6, 9, 13, 15, 17, 25, 27

- pathview, 8, 13, 17, 19, 19, 27
- pathview-package, 2

- reaction2edge, 17
- reaction2edge (combineKEGGnodes), 3
- rn.list (cpd.accs), 4

- sim.mol.data, 26
- strfit (wordwrap), 28

wordwrap, 28