Package 'KEGGprofile'

April 5, 2014

Type Package

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value

Description

The function will transfer a numeric matrix into a matrix of colors, in which the colors represent the values of numeric matrix

Usage

```
col_by_value(x, col, range = NA, breaks = NA)
```

Arguments

X	a numeric matrix
col	colors used to represent the values. (See also 'Details')
range	values out of the range will be modified to in the range.
breaks	a numeric vector of three or more cut points giving the number of intervals into

a numeric vector of three or more cut points giving the number of intervals into

which x is to be cut. See also 'Details'

Details

A colorbar would also be ploted. The returned colors of the function can be used in function plot_profile. if breaks not equal to NA, col must have the same length with breaks-1.

Value

a matrix equal to x, but the values were instead by colors.

Examples

```
data(pho_sites_count)
col < -col_by_value(pho_sites_count, col=colorRampPalette(c(white, khaki2))(4), breaks=c(0,1,4,10,Inf))
```

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Description

The function download XML files and png files from KEGG website to local disk

Usage

```
download_KEGGfile(pathway_id = "00010", specis = "hsa",
  target_dir = getwd())
```

Arguments

pathway_id the KEGG pathway id, such as '00010'

specis the specis id in KEGG database, 'hsa' means human, 'mmu' means mouse, 'rno'

means rat, etc

target_dir the local directory where the downloaded files are saved

Details

If pathway_id is set as 'all', all KEGG pathway ids in KEGG.db package will be used and downloaded from KEGG website

Examples

```
download_KEGGfile(pathway_id="00010",specis=hsa)
```

```
{\tt find\_enriched\_pathway} \ \ \textit{find\_enriched\_pathway}
```

Description

The function will map the genes in KEGG pathway database, and then hypergegeometric tests would be used to estimate the significance of enrichment for each pathway

Usage

```
find_enriched_pathway(gene, specis = "hsa",
  returned_pvalue = 0.05, returned_genenumber = 5)
```

parse_XMLfile

Arguments

gene a numeric matrix

returned_pvalue

the minimum p value for enriched pathways

returned_genenumber

the minimum number of annotated genes for enriched pathways

specis the specis id in KEGG database, 'hsa' means human, 'mmu' means mouse, 'rno'

means rat, etc

Details

Only the pathways with p value <= returned_pvalue in hypergegeometric tests and number of annotated genes >= returned_genenumber would be taken as enriched and returned.

Value

a list with two parts

name stastic description a matirx containing the pathway IDs of enriched pathways, and their

names, p values, number of annotated genes

name detail description a list with the genes annotated for each pathway

Examples

```
data(pho_sites_count)
#the 300 genes with most phospholation sites quantified
genes<-names(rev(sort(pho_sites_count[,1]))[1:300])
pho_KEGGresult<-find_enriched_pathway(genes,specis=hsa)</pre>
```

parse_XMLfile

parse_XMLfile

Description

The function parses KEGG XML (KGML) files

Usage

```
parse_XMLfile(pathway_id, specis, database_dir = getwd())
```

Arguments

 ${\tt database_dir} \qquad \text{the directory where the XML files and png files are located}$

pathway_id the KEGG pathway id, such as '00010'

specis the specis id in KEGG database, 'hsa' means human, 'mmu' means mouse, 'rno'

means rat, etc

pho_sites_count 5

Details

This function will parse the KEGG XML (KGML) file. Then a matrix with genes in this pathway and related infomations will be returned. This matrix can be used for plot the expression profiles on the pathway figure.

Value

a matrix containing genes in this pathway, and their names, locations etc, which could be used in the function plot_profile as param KEGG_database

Examples

XML2database<-parse_XMLfile(pathway_id="04110", specis="hsa", database_dir=system.file("extdata", package="KEGGpr

pho_sites_count

number of phosphorylation sites quantified for each gene

Description

This data set is a data.frame with number of phosphorylation sites quantified for each gene in the analysis.

Source

Olsen, J.V., et al. (2010) Quantitative phosphoproteomics reveals widespread full phosphorylation site occupancy during mitosis, Sci Signal, 3, ra3.

plot_pathway

plot_pathway

Description

A wrapper for function download_KEGGfile, parse_XMLfile and plot_profile

Usage

```
plot_pathway(gene_expr, line_col, groups,
  pathway_id = "00010", specis = "hsa", pathway_min = 5,
  database_dir = getwd(), ...)
```

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Arguments

	any other Arguments for function plot_profile
gene_expr	the matrix for gene expression, row.names should be NCBI gene ID, such as $67040,93683$
line_col	line color for expression in different samples in the pathway map, valid when type='lines'
groups	a character used to indicate expression values from different samples
specis	the specis id in KEGG database, 'hsa' means human, 'mmu' means mouse, 'rno' means rat, etc $$
pathway_min	The pathways with number of annotated genes less than pathway_min would be ignored
database_dir	the directory where the XML files and png files are located
pathway_id	the KEGG pathway id, such as '00010'

Details

This wrapper function is developed to make the visualization process more easier. Firstly the existence of XML file and png file would be checked, if not, the download_KEGGfile function would be used to download the files. Then the parse_XMLfile function would be used to parse the XML file. At last the plot_profile function would be used to generate the pathway map.

See Also

```
download_KEGGfile, parse_XMLfile, plot_profile
```

Examples

```
data(pro_pho_expr)
data(pho_sites_count)
#type=lines
col<-col_by_value(pho_sites_count,col=colorRampPalette(c(white,khaki2))(4),breaks=c(0,1,4,10,Inf))
temp<-plot_pathway(pro_pho_expr,bg_col=col,line_col=c("brown1","seagreen3"),groups=c(rep("Proteome ",6),rep("Pl
#type=bg
pho_expr<-pro_pho_expr[,7:12]
temp<-apply(pho_expr,1,function(x) length(which(is.na(x))))
pho_expr<-pho_expr[which(temp==0),]
col<-col_by_value(pho_expr,col=colorRampPalette(c(green,black,red))(1024),range=c(-6,6))
temp<-plot_pathway(pho_expr,type="bg",bg_col=col,text_col="white",magnify=1.2,specis=hsa,database_dir=system.f</pre>
```

Description

The function plot gene expression profiles on KEGG pathway maps

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Usage

```
plot_profile(gene_expr, pathway_name, KEGG_database,
  groups, bg_col = "white", text_col = "black", line_col,
  border_col = "grey", text_cex = 0.25, magnify = 1,
  type = c("lines", "bg"), pathway_min = 5,
  genes_kept = c("foldchange", "first", "random", "var", "abs"),
  specis = "hsa", database_dir = getwd(), max_dist,
  lwd = 1.2)
```

Arguments

gene_expr the matrix for gene expression, row.names should be NCBI gene ID, such as

67040, 93683

pathway_name the specis id and KEGG pathway id, such as 'hsa00010'

KEGG_database the matrix returned by function parse_XMLfile, which contains genes in this

pathway, and their names, locations etc

groups a character used to indicate expression values from different samples

bg_col background color for gene rectangles in the pathway map

line_col line color for expression in different samples in the pathway map, valid when

type='lines'

text_col the colors for text in the pathway map. A color matrix generated by function

col_by_value can be used here

border_col border color for gene rectangles in the pathway map. A color matrix generated

by function col_by_value can be used here

text_cex cex for text in the pathway map. A color matrix generated by function col_by_value

can be used here

magnify the coefficient used to magnify the gene rectangles

type the type of pathway map visulization, could be 'bg' or 'lines'. Default is 'bg'.

See also 'Details'

pathway_min The pathways with number of annotated genes less than pathway_min would be

ignored

genes_kept methods used for choosing genes when several genes corresponding to one loca-

tion in pathway map. Default is 'foldchange', which kept the gene with largest fold changes. 'first' kept the first gene. 'random' chosed gene random. 'var' kept the gene with largest variation. 'abs' kept the gene with largest absolute

value

max_dist The expression changes that represented by the distance from the bottom to the

top of gene rectangle, valid when type='lines'. This param is used to ensure the dynamic changes of lines in different gene polygon represent equal variation. It would be calculated from the maximum changes of genes in this pathway by default. If max_dist=NA, then the lines would be plotted from top to bottom in

each gene rectangle

1wd The line width when type='lines'

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specis the specis id in KEGG database, 'hsa' means human, 'mmu' means mouse, 'rno'

means rat, etc

database_dir the directory where the XML files and png files are located

Details

There are two visualization methods to represent gene expression profiles: 'background' and 'lines'. The first one is applicable for analysis with only one sample or one type of data, which divides the gene polygon into several sub-polygons to represent different time points. And each sub-polygon has a specific background color to represent expression changes in that time point. The second method plots lines with different colors in the gene polygon to represent different samples or different types of data. The dynamic changes of lines mean the profiles of genes in different time points.

Value

a matrix containing genes maped in this pathway, and their names, expressions

Examples

 $\label{lem:lem:main} $$ XML2 database < -parse_XMLfile(pathway_id="04110", specis="hsa", database_dir=system.file("extdata", package="KEGGpr data(pro_pho_expr)) $$ $$ data(pro_pho_expr) $$ $$ All the proof of th$

 $temp <-plot_profile (pro_pho_expr,pathway_name="hsa04110", KEGG_database=XML2database, line_col=c ("brown1", "seagregated by the color of the colo$

pro_pho_expr

expression profiles in proteome and phosphoproteome

Description

This data set is from a previously published data of proteome and phosphoproteome analysis in different cell phase. The column 1-6 are proteome data and column 7-12 are phosphoproteome data in this data frame. The 6 time points are G1, G1/S, Early S, Late S, G2, Mitosis.

Source

Olsen, J.V., et al. (2010) Quantitative phosphoproteomics reveals widespread full phosphorylation site occupancy during mitosis, Sci Signal, 3, ra3.

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