Package 'PinPath'

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Type Package

Title Visualization of Omics Data onto Pathway Diagrams

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Description PinPath enables flexible visualization of (omics) data onto pathways diagrams, allowing users to pinpoint where the relevant changes occur.
It supports pathway diagrams from WikiPathways and KEGG, as well as custom GPML and KGML files. Data can be displayed on both native pathway layouts and network representations.

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URL https://github.com/SyNUM-lab/PinPath

BugReports https://github.com/SyNUM-lab/PinPath/issues

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`defaultColorList` *Make default colorList*

Description

This function makes default list that can be used to set the node colors in the pathway diagram.

Usage

```
defaultColorList(ColorVar, ColorNames = NULL)
```

Arguments

`ColorVar`	`vector` or `data.frame` for coloring the nodes in the pathway. This can be for instance a `data.frame` with the log2FCs and significance in the columns.
`ColorNames`	(optional) `character` vector with names of the color variables. These will be used to set the names in the legend. If `colorNames` is NULL, the column names of the `colorVar` `data.frame` will be used.

Details

For both divergent and sequential color scales, values outside the specified range (`minVal` to `maxVal`) are clipped and mapped to the colors corresponding to the minimum (`minCol`) or maximum (`maxCol`).

Value

A list that can be provided to drawGPML to set the node colors in the pathway diagram.

Examples

```
# Load example data
lung_expr <- read.csv(system.file(
    "extdata","data-lung-cancer.csv", package="PinPath"),
    stringsAsFactors = FALSE)

# Set significance as a binary variable
lung_expr$Significant <- ifelse(lung_expr$adj.P.Value < 0.05, "Yes", "No")

# Make default color list
colorList <- PinPath::defaultColorList(
lung_expr[,c("log2FC", "Significant")])
```

`drawGPML` *Draw pathway from GPML file*

Description

This function draws a pathway from a GPML file with the option to map, e.g., expression data onto the pathway diagram.

Usage

```
drawGPML(
  infile,
  outdir = getwd(),
  outname = NULL,
  featureIDs = NULL,
  colorVar = NULL,
  annGenes = NULL,
  annMetabolites = NULL,
  inputDB = NULL,
  colorNames = NULL,
  colorList = NULL,
  NAvalue = "#F0F0F0",
  multiMapping = TRUE,
  legend = FALSE,
  nodeTable = FALSE,
  pathInfo = FALSE,
  openFile = FALSE
)
```

Arguments

`infile`	Input GPML file. This can be a character string of the GPML file location (e.g., "Downloads/WP42500.gpml") or a GPML string provided by [rWikiPathways::getPathway].
`outdir`	(optional) Output directory. The pathway and legend images will be saved in this directory.

outname	(optional) The file name of the output pathway image. "svg","png",and "pdf" file extensions are accepted. If no file extension is specified, the pathway and legend image will be generated in .svg format. The legend file gets the "legend_" prefix.
featureIDs	(optional) character vector of feature IDs.
colorVar	(optional) vector or data.frame for coloring the nodes in the pathway. This can be for instance a data.frame with the log2FCs and significance in the columns. The (row) order should match featureIDs. The color rules and palettes for the supplied values can be set in the colorList parameter.
annGenes	(optional) character string of the Bioconductor annotation package (e.g., org.Hs.eg.db).
annMetabolites	(optional) tibble or data.frame with metabolite mapping information (see metaboliteIDmapping package).
inputDB	(optional) Input gene ID type (SYMBOL, ENTREZID, ENSEMBL, UNIPROT). This can be a character vector of length = 1 (if all gene IDs are of the same type) or of length = nrow(featureIDs) (if you want to specify the type per gene ID).
colorNames	(optional) character vector with names of the color variables. If colorNames is NULL, the column names of the colorVar data.frame will be used.
colorList	(optional) A list with information about the coloring of the nodes. An example can be generated using the defaultColorList function.
NAvalue	(optional) Node color for NA values.
multiMapping	(optional) Logical (TRUE or FALSE). If a node has multiple feature IDs, should all associated values be plotted? If FALSE, only the value of the first feature ID is plotted.
legend	(optional) Logical (TRUE or FALSE). Should the legend be plotted?
nodeTable	(optional) Logical (TRUE or FALSE). Should a node table be returned?
pathInfo	(optional) Logical (TRUE or FALSE). Should pathway information be returned?
openFile	(optional) Logical (TRUE or FALSE). Should the pathway file be opened after it has been saved? This option only works for Windows users.

Value

A list with the node table and the file location of the pathway and legend image.

Examples

```
# Load example data
lung_expr <- read.csv(system.file(
    "extdata","data-lung-cancer.csv", package="PinPath"),
    stringsAsFactors = FALSE)

# Select pathway
infile <- rWikiPathways::getPathway("WP4255")

# Draw pathway
pathVis <- PinPath::drawGPML(
    infile = infile,
    outdir = tempdir(),
    annGenes = "org.Hs.eg.db",
    inputDB = "ENSEMBL",
```

```
    featureIDs = lung_expr$GeneID,
    colorVar = lung_expr[,"log2FC"],
    nodeTable = TRUE,
    legend = TRUE,
    openFile = FALSE) # <-- set to TRUE to open the image automatically
```

---

drawKGML *Draw pathway from KGML file*

Description

This function draws a pathway from a KGML file with the option to map, e.g., expression data onto the pathway diagram.

Usage

```
drawKGML(
  infile,
  outdir = getwd(),
  outname = NULL,
  annGenes = NULL,
  annMetabolites = NULL,
  inputDB = NULL,
  featureIDs = NULL,
  colorVar = NULL,
  colorNames = NULL,
  colorList = NULL,
  NAvalue = "#F0F0F0",
  multiMapping = TRUE,
  legend = FALSE,
  nodeTable = FALSE,
  pathInfo = FALSE,
  openFile = FALSE
)
```

Arguments

infile	Input KGML file. This can be a character string of the KGML file location (e.g., "Downloads/WP42500.KGML").
outdir	(optional) Output directory. The pathway and legend images will be saved in this directory.
outname	(optional) The file name of the output pathway image. "svg","png",and "pdf" file extensions are accepted. If no file extension is specified, the pathway and legend image will be generated in .svg format. The legend file gets the "legend_" prefix.
annGenes	(optional) `character` string of the Bioconductor annotation package (e.g., org.Hs.eg.db).
annMetabolites	(optional) `tibble` or `data.frame` with metabolite mapping information (see metaboliteIDmapping package).

inputDB	(optional) Input gene ID type (SYMBOL, ENTREZID, ENSEMBL, UNIPROT). This can be a character vector of length = 1 (if all gene IDs are of the same type) or of length = nrow(featureIDs) (if you want to specify the type per gene ID).
featureIDs	(optional) character vector of feature IDs.
colorVar	(optional) vector or data.frame for coloring the nodes in the pathway. This can be for instance a data.frame with the log2FCs and significance in the columns. The (row) order should match featureIDs. The color rules and palettes for the supplied values can be set in the colorList parameter.
colorNames	(optional) character vector with names of the color variables. If colorNames is NULL, the column names of the colorVar data.frame will be used.
colorList	(optional) A list with information about the coloring of the nodes. An example can be generated using the defaultColorList function.
NAvalue	(optional) Node color for NA values.
multiMapping	(optional) Logical (TRUE or FALSE). If a node has multiple feature IDs, should all associated values be plotted? If FALSE, only the value of the first feature ID is plotted.
legend	(optional) Logical (TRUE or FALSE). Should the legend be plotted?
nodeTable	(optional) Logical (TRUE or FALSE). Should a node table be returned?
pathInfo	(optional) Logical (TRUE or FALSE). Should pathway information be returned?
openFile	(optional) Logical (TRUE or FALSE). Should the pathway file be opened after it has been saved? This option only works for Windows users.

Value

A list with the node table and the file location of the pathway and legend image.

Examples

```
# Load example data
lung_expr <- read.csv(system.file(
    "extdata","data-lung-cancer.csv", package="PinPath"),
    stringsAsFactors = FALSE)

# Select pathway
pathway_id <- "hsa05223"
bfc <- BiocFileCache::BiocFileCache()
infile <- BiocFileCache::bfcrpath(bfc,
paste0("https://rest.kegg.jp/get/",pathway_id,"/kgml"))

# Draw pathway
pathVis <- PinPath::drawKGML(
    infile = infile,
    outdir = tempdir(),
    annGenes = "org.Hs.eg.db",
    inputDB = "ENSEMBL",
    featureIDs = lung_expr$GeneID,
    colorVar = lung_expr[,"log2FC"],
    nodeTable = TRUE,
    legend = TRUE,
    openFile = FALSE) # <-- set to TRUE to open the image automatically
```

`GPML2Network` *Draw network from GPML file*

Description

This function draws a network from a GPML file with the option to map, e.g., expression data onto the network diagram.

Usage

```
GPML2Network(
  infile,
  outdir = getwd(),
  outname = NULL,
  featureIDs = NULL,
  colorVar = NULL,
  annGenes = NULL,
  annMetabolites = NULL,
  inputDB = NULL,
  colorNames = NULL,
  colorList = NULL,
  NAvalue = "#F0F0F0",
  layout = "nicely",
  unconnectedNodes = FALSE,
  alpha = 0.9,
  nodeSize = 1,
  fontSize = 2,
  legend = FALSE,
  nodeTable = FALSE,
  pathInfo = FALSE,
  openFile = FALSE
)
```

Arguments

`infile`	Input GPML file. This can be a character string of the GPML file location (e.g., "Downloads/WP42500.gpml") or a GPML string provided by [rWikiPathways::getPathway].
`outdir`	(optional) Output directory. The pathway and legend images will be saved in this directory.
`outname`	(optional) The file name of the output pathway image. "svg","png",and "pdf" file extensions are accepted. If no file extension is specified, the pathway and legend image will be generated in .svg format. The legend file gets the "legend_" prefix.
`featureIDs`	(optional) `character` vector of gene IDs.
`colorVar`	(optional) `vector` or `data.frame` for coloring the nodes in the pathway. This can be for instance a `data.frame` with the log2FCs and significance in the columns. The (row) order should match `featureIDs`. The color rules and palettes for the supplied values can be set in the colorList parameter.

annGenes	(optional) character string of the Bioconductor annotation package (e.g., org.Hs.eg.db).
annMetabolites	(optional) tibble or data.frame with metabolite mapping information (see metaboliteIDmapping package).
inputDB	(optional) Input gene ID type (SYMBOL, ENTREZID, ENSEMBL, UNIPROT). This can be a character vector of length = 1 (if all gene IDs are of the same type) or of length = nrow(featureIDs) (if you want to specify the type per gene ID).
colorNames	(optional) character vector with names of the color variables. If colorNames is NULL, the column names of the colorVar data.frame will be used.
colorList	(optional) A list with information about the coloring of the nodes. An example can be generated using the defaultColorList function.
NAvalue	(optional) Node color for NA values.
layout	(optional) Network layout from igraph.
unconnectedNodes	(optional) Logical (TRUE or FALSE). Should unconnected (isolated) nodes be shown in the network?
alpha	(optional) Transparency of the nodes.
nodeSize	(optional) Size of the nodes.
fontSize	(optional) Font size of the text in the nodes.
legend	(optional) Logical (TRUE or FALSE). Should the legend be plotted?
nodeTable	(optional) Logical (TRUE or FALSE). Should a node table be returned?
pathInfo	(optional) Logical (TRUE or FALSE). Should pathway information be returned?
openFile	(optional) Logical (TRUE or FALSE). Should the pathway file be opened after it has been saved? This option only works for Windows users.

Value

A list with the node table and the file location of the pathway and legend image.

Examples

```
# Load example data
lung_expr <- read.csv(system.file(
    "extdata","data-lung-cancer.csv", package="PinPath"),
    stringsAsFactors = FALSE)

# Select pathway
infile <- rWikiPathways::getPathway("WP4255")

# Draw pathway
pathVis <- PinPath::GPML2Network(
    infile = infile,
    outdir = tempdir(),
    annGenes = "org.Hs.eg.db",
    inputDB = "ENSEMBL",
    featureIDs = lung_expr$GeneID,
    colorVar = lung_expr[,"log2FC"],
    nodeTable = TRUE,
    legend = TRUE,
    openFile = FALSE) # <-- set to TRUE to open the image automatically
```

KGML2Network *Draw network from KGML file*

Description

This function draws a pathway from a KGML file with the option to map, e.g., expression data onto the pathway diagram.

Usage

```
KGML2Network(
  infile,
  outdir = getwd(),
  outname = NULL,
  featureIDs = NULL,
  colorVar = NULL,
  annGenes = NULL,
  annMetabolites = NULL,
  inputDB = NULL,
  colorNames = NULL,
  colorList = NULL,
  NAvalue = "#F0F0F0",
  layout = "nicely",
  unconnectedNodes = FALSE,
  alpha = 0.9,
  nodeSize = 1,
  fontSize = 2,
  legend = FALSE,
  nodeTable = FALSE,
  pathInfo = FALSE,
  openFile = FALSE
)
```

Arguments

infile	Input KGML file. This can be a character string of the KGML file location (e.g., "Downloads/WP42500.KGML").
outdir	(optional) Output directory. The pathway and legend images will be saved in this directory.
outname	(optional) The file name of the output pathway image. "svg","png",and "pdf" file extensions are accepted. If no file extension is specified, the pathway and legend image will be generated in .svg format. The legend file gets the "legend_" prefix.
featureIDs	(optional) `character` vector of gene IDs.
colorVar	(optional) `vector` or `data.frame` for coloring the nodes in the pathway. This can be for instance a `data.frame` with the log2FCs and significance in the columns. The (row) order should match `featureIDs`. The color rules and palettes for the supplied values can be set in the colorList parameter.
annGenes	(optional) `character` string of the Bioconductor annotation package (e.g., org.Hs.eg.db).

annMetabolites	(optional) tibble or data.frame with metabolite mapping information (see metaboliteIDmapping package).
inputDB	(optional) Input gene ID type (SYMBOL, ENTREZID, ENSEMBL, UNIPROT). This can be a character vector of length = 1 (if all gene IDs are of the same type) or of length = nrow(featureIDs) (if you want to specify the type per gene ID).
colorNames	(optional) character vector with names of the color variables. If colorNames is NULL, the column names of the colorVar data.frame will be used.
colorList	(optional) A list with information about the coloring of the nodes. An example can be generated using the defaultColorList function.
NAvalue	(optional) Node color for NA values.
layout	(optional) Network layout from igraph.
unconnectedNodes	(optional) Logical (TRUE or FALSE). Should unconnected (isolated) nodes be shown in the network?
alpha	(optional) Transparency of the nodes.
nodeSize	(optional) Size of the nodes.
fontSize	(optional) Font size of the text in the nodes.
legend	(optional) Logical (TRUE or FALSE). Should the legend be plotted?
nodeTable	(optional) Logical (TRUE or FALSE). Should a node table be returned?
pathInfo	(optional) Logical (TRUE or FALSE). Should pathway information be returned?
openFile	(optional) Logical (TRUE or FALSE). Should the pathway file be opened after it has been saved? This option only works for Windows users.

Value

A list with the node table and the file location of the pathway and legend image.

Examples

```
# Load example data
lung_expr <- read.csv(system.file(
    "extdata","data-lung-cancer.csv", package="PinPath"),
    stringsAsFactors = FALSE)

# Select pathway
pathway_id <- "hsa05223"
bfc <- BiocFileCache::BiocFileCache()
infile <- BiocFileCache::bfcrpath(bfc,
paste0("https://rest.kegg.jp/get/",pathway_id,"/kgml"))

# Draw pathway
pathVis <- PinPath::KGML2Network(
    infile = infile,
    outdir = tempdir(),
    annGenes = "org.Hs.eg.db",
    inputDB = "ENSEMBL",
    featureIDs = lung_expr$GeneID,
    colorVar = lung_expr[,"log2FC"],
    nodeTable = TRUE,
    legend = TRUE,
```

```
        openFile = FALSE) # <-- set to TRUE to open the image automatically
```

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