

Package ‘SBGNview’

October 7, 2023

Title ``SBGNview: Data Analysis, Integration and Visualization on SBGN Pathways"

Description SBGNview is a tool set for pathway based data visualization, integration and analysis. SBGNview is similar and complementary to the widely used Pathview, with the following key features:
1. Pathway definition by the widely adopted Systems Biology Graphical Notation (SBGN); 2. Supports multiple major pathway databases beyond KEGG (Reactome, MetaCyc, SMPDB, PANTHER, METACROP) and user defined pathways; 3. Covers 5,200 reference pathways and over 3,000 species by default; 4. Extensive graphics controls, including glyph and edge attributes, graph layout and sub-pathway highlight; 5. SBGN pathway data manipulation, processing, extraction and analysis.

Version 1.14.0

Author Xiaoxi Dong*, Kovidh Vegesna*, Weijun Luo

Maintainer Weijun Luo <luo_weijun@yahoo.com>

Depends R (>= 3.6), pathview, SBGNview.data

Imports Rdpack, grDevices, methods, stats, utils, xml2, rsvg, igraph, rmarkdown, knitr, SummarizedExperiment, AnnotationDbi, httr, KEGGREST, bookdown

RdMacros Rdpack

License AGPL-3

LazyData FALSE

Collate SBGN.to.SVG.R SBGNview.R SBGNview.obj.fun.R color.panel.R data.R download.utilities.R highlight.utilities.R mapping.utilities.R parsing.utilities.R plot.utilities.R zzz.R

RoxygenNote 7.1.1

Suggests testthat, gage

VignetteBuilder knitr

Encoding UTF-8

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

URL <https://github.com/dataplab/SBGNview>

BugReports <https://github.com/dataplab/SBGNview/issues>

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

git_branch RELEASE_3_17

git_last_commit e64acdb

git_last_commit_date 2023-04-25

Date/Publication 2023-10-06

R topics documented:

+.SBGNview	3
arc-class	3
changeDataId	4
changeIds	6
downloadSbgnFile	7
findPathways	8
glyph-class	9
highlightArcs	10
highlightNodes	11
highlightPath	12
loadMappingTable	14
mapped.ids	15
outputFile	16
outputFile<-	16
pathways.info	17
pathways.stats	17
print.SBGNview	18
renderSbgn	19
sbgn.gsets	24
SBGNhub.id.mapping.tables	25
sbgnNodes	26
SBGNview	27
spline.arc-class	33
Index	35

+.SBGNview	<i>Generic function to modify SBGN graph features</i>
------------	---

Description

This binary operator ('+') modifies a SBGNview object(first argument) using a function (second argument)

Usage

```
## S3 method for class 'SBGNview'
SBGNview.obj + fn
```

Arguments

SBGNview.obj	An object of class SBGNview
fn	A character string. The name of any funtion that modifies and returns a SBGN-view object. Some functions are available in SBGNview package: highlightPath , highlightNodes .

Value

The returned value of *fn*

Examples

```
## Not run:
obj.new <- SBGNview.obj + highlightArcs(class = 'production',
                                       color = 'red')

## End(Not run)
```

arc-class	<i>An object to store arc information</i>
-----------	---

Description

An object to store arc information

Details

Information in an 'arc' object comes from two sources: 1. SBGN-ML file's 'arc' element ('source', 'target', coordinates etc.). 2. Parameters specified when running function [SBGNview](#). User can modify arc objects to change the way how they are rendered. See the "arcs.user" argument in [renderSbgn](#).

Slots

- `target`, `source`, `id`, `arc.class` A character string. Information extracted from element 'arc'.
- `start.x`, `start.y`, `end.x`, `end.y` Numeric. Information extracted from elements 'start', 'end' or 'next'.
- `stroke.opacity` Numeric. Controls the line of an arc (not tip of the arc).
- `parameters.list` A list. The `parameters.list` slot is a copy of the `global.parameters.list`. The `global.parameters.list` contains the '...' parameters passed into `SBGNview` which will be used by `renderSbgn`. By default this slot for all arc objects in the output `SBGNview` object will be an empty list. You can add named elements to this slot to customize each individual arc. For information about which parameters can be set in the `parameters.list` slot, see the arguments in `renderSbgn`. A customized list of arc objects can be passed as input into `SBGNview` function using the 'arcs.user' argument (see `renderSbgn` for more information).
- `edge` A list. An arc in SBGN map normally consists of a line and a tip at the end of the line. This list holds variables that controls arc properties. Available elements can be accessed as follow:
The following three parameters control the line:
`arc@edge$line.stroke.color`
`arc@edge$line.stroke.opacity`
`arc@edge$line.width`
- The following five parameters control the tip:
`arc@edge$tip.stroke.opacity`
`arc@edge$tip.stroke.color`
`arc@edge$tip.stroke.width`
`arc@edge$tip.fill.color`
`arc@edge$tip.fill.opacity`

 changeDataId

Change the data IDs of input omics data matrix

Description

This function changes the IDs of input omics data from one type to another. It returns a data matrix with row names changed to the specified output ID type. To change a vector of input IDs to another type, use the `changeIds` function.

Usage

```
changeDataId(
  data.input.id = NULL,
  input.type = NULL,
  output.type = NULL,
  sum.method = "sum",
  org = "hsa",
  mol.type = NULL,
```

```

    id.mapping.table = NULL,
    SBGNview.data.folder = "./SBGNview.tmp.data"
)

```

Arguments

<code>data.input.id</code>	A matrix. Input omics data. Rows are genes or compounds, columns are measurements. Row names are the original IDs that need to be transformed.
<code>input.type</code>	A character string. The type of input IDs. Please check <code>data('mapped.ids')</code> for supported types.
<code>output.type</code>	A character string. The type of output IDs. Please check <code>data('mapped.ids')</code> for supported types.
<code>sum.method</code>	A character string. Default: "sum". In some cases multiple input IDs are mapped to one output ID. In this situation, we may need to derive only one value from them. This parameter is a function that can derive a single numeric value from a vector of numeric values (e.g. 'sum','max','min','mean'), including a User Defined Function (UDF).
<code>org</code>	A character string. Default: "hsa". The species source of omics data. 'changeDataId' uses pathview to map between some gene ID types. Please use '?geneannot.map' to check the detail. Pathview needs species information to do the job. This parameter is a two-letter abbreviation of organism name, or KEGG species code, or the common species name, used to determine the gene annotation package. For all potential values check: <code>data(bods)</code> ; <code>bods</code> . Default <code>org='Hs'</code> , and can also be 'hsa' or 'human' (case insensitive).
<code>mol.type</code>	A character string. Either 'cpd' or 'gene' – the type of input omics data.
<code>id.mapping.table</code>	A matrix. Mapping table between <code>input.type</code> and <code>output.type</code> . This matrix should have two columns for <code>input.type</code> and <code>output.type</code> , respectively. Column names should be the values of parameters 'input.type' and 'output.type'. See example section for an example.
<code>SBGNview.data.folder</code>	A character string. Default: "./SBGNview.tmp.data". The path to a folder that will hold downloaded ID mapping files and pathway information data files.

Details

This function maps between various gene/compound ID types.

1. Map other ID types to glyph IDs in SBGN-ML files of pathwayCommons database, and MetaCyc database: Use `output.type = 'pathwayCommons'` or `output.type = 'metacyc.SBGN'`. Please check `data('mapped.ids')` for supported input ID types.

2. Map between other ID types:

- 2.1 ID types pairs can be mapped by pathview. Currently SBGNview uses pathview to do this mapping. Please check pathview functions 'geneannot.map' and 'cpdidmap' for more details.

- 2.2 Other ID type pairs

In this case, users need to provide `id.mapping.table`.

Value

A matrix, row names are changed to IDs of 'output.type'. Note the number of rows may be different from input matrix, because multiple input IDs could be collapsed to a single output ID. Also a single input ID could map to multiple output IDs.

Examples

```
# Change gene ID
data(mapped.ids)
library(pathview)
data('gse16873.d')
gene.data = gse16873.d[c('7157', '1032'),]
mapping.table = data.frame(ENTREZID = c('7157', '1032'),
                           SYMBOL = c('TP53', 'CDKN2D'),
                           stringsAsFactors = FALSE)
new.dt = changeDataId(data.input.id = gene.data,
                      output.type = 'SYMBOL',
                      input.type = 'ENTREZID',
                      mol.type = 'gene',
                      id.mapping.table = mapping.table)
```

changeIds

Change vector of input IDs to another ID type

Description

This function changes a vector of input IDs to another ID type. It returns a list where each element is the input ID type is mapped to the output ID type. Please note that not every input ID might be mapped to the output type. To change the input IDs to another ID type for a data matrix, use the [changeDataId](#) function.

Usage

```
changeIds(
  input.ids = NULL,
  input.type = NULL,
  output.type = NULL,
  mol.type = NULL,
  limit.to.pathways = NULL,
  org = "hsa",
  SBGNview.data.folder = "./SBGNview.tmp.data"
)
```

Arguments

<code>input.ids</code>	A vector of character strings. Input IDs that need to be converted.
<code>input.type</code>	A character string. The type of input IDs. Supported ID types can be found in <code>data(mapped.ids)</code>
<code>output.type</code>	A character string. The type of output IDs. Supported ID types can be found in <code>data(mapped.ids)</code>
<code>mol.type</code>	A character string. One of 'gene' or 'cpd'.
<code>limit.to.pathways</code>	A vector of character strings. A vector of pathways IDs. When 'output.type' is one of 'pathwayCommons' or 'metacyc.SBGN', one input ID (e.g. gene symbol) can map to multiple nodes in different pathways (SBGN-ML files). In this case, we can limit output to the specified pathways. When 'output.type' is NOT one of 'pathwayCommons' or 'metacyc.SBGN', this argument is ignored.
<code>org</code>	A character string. Default: "hsa". Three letter KEGG species code.
<code>SBGNview.data.folder</code>	A character string. Default: "./SBGNview.tmp.data". The path to a folder that will hold downloaded ID mapping files and pathway information data files.

Value

A list. Each element is the IDs in `output.type` that are mapped to one input ID.

Examples

```
data(mapped.ids)
mapping <- changeIds(input.ids = c(10327, 6652),
                    input.type = 'ENTREZID',
                    output.type = 'pathwayCommons',
                    mol.type = 'gene',
                    org = "hsa")
```

`downloadSbgnFile`

Download pre-generated SBGN-ML file from GitHub

Description

This function will download a SBGN-ML file from our pre-collected SBGN-ML files given the 'pathway.id' argument.

Usage

```
downloadSbgnFile(pathway.id, download.folder = "./")
```

Arguments

`pathway.id` A character string. The ID of pathway. For accepted pathway IDs, please check `data('pathways.info')`. IDs are in column 'pathway.id' (`pathways.info[, 'pathway.id']`)

`download.folder` A character string. Default: `"/"`. The output folder to store created SBGN-ML files.

Value

A vector of character strings. The path to the created SBGN-ML files.

Examples

```
data("pathways.info")
data("sbgn.xmls")
input.sbn <- downloadSbnFile(pathway.id = pathways.info[1, 'pathway.id'],
                             download.folder = './')
```

<code>findPathways</code>	<i>Retrieve pathways by keywords</i>
---------------------------	--------------------------------------

Description

This function searches for pathways by input keywords.

Usage

```
findPathways(
  keywords = NULL,
  keywords.logic = "or",
  keyword.type = "pathway.name",
  org = NULL,
  SBGNview.data.folder = "./SBGNview.tmp.data"
)
```

Arguments

`keywords` A character string or vector. The search is case in-sensitive.

`keywords.logic` A character string. Options are 'and' or 'or' (default). This will tell the function if the search require 'all' or 'any' of the keywords to be present. It only makes difference when `keyword.type` is 'pathway.name'.

`keyword.type` A character string. Either 'pathway.name' (default) or one of the ID types in `data('mapped.ids')`

`org` A character string. The KEGG species code.

`SBGNview.data.folder` A character string. Default: `"/SBGNview.tmp.data"`. The path to a folder that will hold downloaded ID mapping files and pathway information data files.

Details

If 'keyword.type' is 'pathway.name' (default), this function will search for the presence of any keyword in the pathway.name column of data(pathways.info). The search is case in-sensitive. If 'keyword.type' is one of the identifier types and 'keywords' are corresponding identifiers, this function will return pathways that include nodes mapped to input identifiers.

Value

A dataframe. Contains information of pathways found.

Examples

```
data(pathways.info)
input.pathways <- findPathways('Adrenaline and noradrenaline biosynthesis')
```

glyph-class

An object to store glyph information

Description

An object to store glyph information

Details

User can modify glyph objects to change the way how they are rendered. See the "glyphs.user" argument in [renderSbgn](#).

Slots

compartment A character string. The compartment this glyph belongs to.

x, y, h, w Numeric. The x,y location and height, width of the glyph.

id A character string. The ID of the glyph (determined by the 'id' attribute in element 'glyph').

label A character string. label of the glyph. Extracted from the element 'label'.

glyph.class A character string. Class of the glyph.

user.data A numeric vector. The omics data mapped to this glyph.

stroke.width, stroke.opacity, fill.opacity Numeric. Controls glyph border width or opacity of node fill and border.

fill.color, stroke.color A character string. The fill color and stroke color of glyph.

label_location A character string. One of 'center' or 'top'. If set to 'center', the glyph label text will be displayed at the center of the glyph. If set to 'top', the label will be displayed at the top of the glyph.

orientation A character string. One of 'left', 'right', 'up', 'down'. This only applies to glyphs of classes 'terminal' and 'tag'. It will change the orientation of the node.

`parameters.list` A list. The `parameters.list` slot is a copy of the `global.parameters.list`. The `global.parameters.list` contains the '...' parameters passed into `SBGNview` which will be used by `renderSbgn`. By default this slot for all glyph objects in the output `SBGNview` object will be an empty list. You can add named elements to this slot to customize each individual glyph. For information about which parameters can be set in the `parameters.list` slot, see the arguments in `renderSbgn`. A customized list of glyph objects can be passed as input into `SBGNview` function using the 'glyphs.user' argument (see `renderSbgn` for more information).

`shape` A list. Parameters controlling how the node is rendered. Available elements can be accessed as follow: `glyph@shape$stroke.color`
 -Character (e.g. 'red'). The color of glyph border.
`glyph@shape$stroke.opacity`
 -Numeric (e.g. 0.8). The opacity of glyph border. Must be between 0 and 1.
`glyph@shape$stroke.width`
 -Numeric. The thickness of glyph border.
`glyph@shape$fill.opacity`
 -Numeric. The opacity of glyph fill. Must be between 0 and 1.
`glyph@shape$fill.color`
 -Numeric. The glyph fill color. Note that this will overwrite colors generated from omics data!

`text` A list. Parameters controlling how node label is rendered. Available elements can be accessed as follow: `glyph@text$y.shift`
 -Numeric. Move glyph label vertically by this value.
`glyph@text$x.shift`
 -Numeric. Move glyph label horizontally by this value.
`glyph@text$color`
 -A character string. The color of glyph label.
`glyph@text$font.size`
 -A character string. The font size of glyph label.

highlightArcs

Highlight arcs by arc class

Description

This function can modify a `SBGNview` object's arc. Normally we use it as an argument to `+.SBGNview` and modify a `SBGNview` object. Run `help("+.SBGNview")` for more information.

Usage

```
highlightArcs(class = "all", color = "black", line.width = 2, tip.size = 6)
```

Arguments

<code>class</code>	A character string. Default: "arc". The arc class to modify.
<code>color</code>	A character string. Default: "black". The color of arcs with selected 'class'.
<code>line.width</code>	Numeric. Default: 2. Line thickness.
<code>tip.size</code>	Numeric. Default: 6. Tip size.

Value

A SBGNview object

Examples

```
## Not run:  
obj.new <- SBGNview.obj + highlightArcs(class = 'production', color = 'red')  
  
## End(Not run)
```

highlightNodes	<i>Highlight input nodes</i>
----------------	------------------------------

Description

Change node properties such as border color and width to highlight a list of input nodes. This function should be used as the second argument to function. Run `help("+.SBGNview")` for more information.

Usage

```
highlightNodes(  
  node.set = "all",  
  node.set.id.type = "compound.name",  
  glyphs.id.type = "pathwayCommons",  
  mol.type = "cpd",  
  stroke.color = "black",  
  stroke.width = 10,  
  stroke.opacity = 1,  
  show.glyph.id = FALSE,  
  select.glyph.class = c(),  
  label.x.shift = 0,  
  label.y.shift = 0,  
  label.color = "black",  
  label.font.size = NULL,  
  label.splitting.string = NULL,  
  labels = NULL  
)
```

Arguments

`node.set` A vector of character strings. Default: "all". Input molecule IDs whose nodes are to be highlighted. It can be any ID types supported by SBGNview.

`node.set.id.type` A character string. Default: "compound.name". ID type of input nodes.

`glyphs.id.type` A character string. Default: "pathwayCommons". ID type of nodes in SBGN-ML file.

mol.type	A character string. One of 'gene' or 'cpd' (default).
stroke.color	A character string. Default: "black". The border color of highlighted nodes.
stroke.width	Integer. Default: 10. The border stroke width of highlighted nodes.
stroke.opacity	Numeric. Default: 1. The border stroke opacity of highlighted nodes.
show.glyph.id	Logical. Default: F. If set to 'TRUE', glyph IDs are plotted instead of their labels.
select.glyph.class	Character vector. Select glyphs by class. It should be one of the values of XML attribute 'class' of a 'glyph' element. For example 'macromolecule', "simple chemical"
label.x.shift	Integer. Default: 0. Move labels horizontally.
label.y.shift	Integer. Default: 0. Move labels vertically.
label.color	A character string. Default: "black". Change label color.
label.font.size	Integer. Adjust label font size.
label.splitting.string	A character vector. When we split text into multiple lines, these characters will be used to split label (where a new line can be created). For example: label.splitting.string = c(' ','-',';','/','_').
labels	A vector of character strings. The labels to display on the nodes of input molecules. The names of this vector should be the vector of 'node.set'. The values are the new labels to display.

Value

A SBGNview obj

Examples

```
## Not run:
obj.new <- SBGNview.obj + highlightNodes(node.set = c('tyrosine', '(+)-epinephrine'),
                                         stroke.width = 4,
                                         stroke.color = 'green')

## End(Not run)
```

highlightPath

Highlight shortest path between two nodes

Description

Given two nodes, find the shortest path between them and highlight the path. Other molecules/nodes and edges involved in reactions in the path are also highlighted. This function should be used as the second argument to function. Run `help("+ .SBGNview")` for more information.

Usage

```
highlightPath(
  from.node = NULL,
  to.node = NULL,
  directed.graph = TRUE,
  node.set.id.type = "compound.name",
  glyphs.id.type = "pathwayCommons",
  mol.type = "cpd",
  input.node.stroke.width = 10,
  from.node.color = "red",
  to.node.color = "blue",
  path.node.color = "black",
  path.node.stroke.width = 10,
  n.shortest.paths.plot = 1,
  shortest.paths.cols = c("purple"),
  path.stroke.width = 2,
  tip.size = 4
)
```

Arguments

`from.node` A character string. The molecule ID of source node.

`to.node` A character string. The molecule ID of target node.

`directed.graph` Logical. If treat the SBGN map as a directed graph. If treat it as directed graph, the direction of an arc is determined by the <arc> XML element in the input SBGN-ML file: from 'source' node to 'target' node.

`node.set.id.type` A character string. Default: "compound.name". ID type of input nodes.

`glyphs.id.type` A character string. Default: "pathwayCommons". ID type of nodes in SBGN-ML file.

`mol.type` A character string. One of 'gene' or 'cpd' (default).

`input.node.stroke.width` Integer. Default: 10. Border stroke width of input nodes (affects both `from.node` and `to.node`)

`from.node.color` A character string. Default: "red". Border color of 'source'/`from.node`

`to.node.color` A character string. Default: "blue". Border color of 'target'/`to.node`

`path.node.color` A character string. Default: "black". Border color of nodes in the path.

`path.node.stroke.width` Integer. Default: 10. Adjust stroke width of path between nodes.

`n.shortest.paths.plot` Integer. Default: 1. There could be more than one shortest paths between two nodes. User can choose how many of them to plot.

`shortest.paths.cols`
 A vector of character string. Default: `c("purple")`. The colors of arcs in different shortest paths. The length of this vector (number of colors) should be the value of `n.shortest.paths.plot`. If one arc is in multiple shortest paths, its color will be set to the color that appears later in this vector.

`path.stroke.width`
 Integer. Default: 2. The width of line in edges in the shortest paths.

`tip.size`
 Integer. Default: 4. The size of arc tip in edges of the shortest paths.

Value

A SBGNview obj

Examples

```
## Not run:
obj.new <- SBGNview.obj + highlightPath(from.node = c('tyrosine'),
                                       to.node = c('dopamine'),
                                       from.node.color = 'red',
                                       to.node.color = 'blue')

## End(Not run)
```

<code>loadMappingTable</code>	<i>Generate ID mapping table from input and output ID types</i>
-------------------------------	---

Description

This function generates the ID mapping table between input and output ID types. If provided a vector of input IDs (`limit.to.ids` argument), the function will output mapping table only containing the input IDs. Otherwise, the function will output all IDs of input and output types (restricted to a species if working on gene types and specified the `'species'` parameter). This function will check if a mapping table exists in local folder (`'SBGNview.data.folder'` argument), `SBGNview.data` package, and `SBGNhub`. If no mapping table is found in these locations, a mapping table is generated using `Pathview` and saved to path specified by `'SBGNview.data.folder'` argument.

Usage

```
loadMappingTable(
  input.type = NULL,
  output.type = NULL,
  species = NULL,
  mol.type = NULL,
  limit.to.ids = NULL,
  SBGNview.data.folder = "./SBGNview.tmp.data"
)
```

Arguments

input.type	A character string. Gene or compound ID type
output.type	A character string. Gene or compound ID type
species	A character string. Three letter KEGG species code.
mol.type	A character string. Either 'gene' or 'cpd'.
limit.to.ids	Vector. Molecule IDs of 'input.type'.
SBGView.data.folder	A character string. Default: "./SBGView.tmp.data". The path to a folder that will hold downloaded ID mapping files and pathway information data files.

Value

A list containing the mapping table.

Examples

```
data(mapped.ids)
entrez.to.pathwayCommons <- loadMappingTable(input.type = 'ENTREZID',
                                             output.type = 'pathwayCommons',
                                             species = 'hsa',
                                             mol.type = 'gene')
```

mapped.ids

IDs mappable by SBGView

Description

IDs mappable by SBGView

Usage

```
data(mapped.ids)
```

Format

A list with two elements: A vector of mappable gene ID types (mapped.ids[["gene"]]), a vector of mappable compound ID types (mapped.ids[["cpd"]]).

Details

ID types mappable to glyph IDs in SBGView SBGView-ML file collection.

outputFile	<i>Retrieve output file information from a SBGNview object</i>
------------	--

Description

Retrieve output file information from a SBGNview object

Usage

```
outputFile(obj)
```

Arguments

obj A SBGNview class object.

Details

This function prints the output file path recorded in a SBGNview object.

Value

A string. The output file information.

Examples

```
## Not run:  
outputFile(SBGNview.obj)  
  
## End(Not run)
```

outputFile<-	<i>Set or change output file information for a SBGNview object</i>
--------------	--

Description

Set or change output file information for a SBGNview object

Usage

```
outputFile(obj) <- value
```

Arguments

obj A SBGNview class object
value No need to provide

Details

This function sets the output file path recorded in a SBGNview object.

Value

A SBGNview class object

Examples

```
## Not run:  
outputFile(SBGNview.obj) <- "test.output.file"  
  
## End(Not run)
```

pathways.info	<i>Information of collected pathways</i>
---------------	--

Description

Information of collected pathways

Usage

```
data(pathways.info)
```

Format

A data.frame

Details

The information of pre-collected pathways and their SBGN-ML file information, such as pathway ID, name, source database, glyph ID types and URLs to the original pathway webpages.

pathways.stats	<i>Number of pathways collected</i>
----------------	-------------------------------------

Description

Number of pathways collected

Usage

```
data(pathways.stats)
```

Format

A data.frame

Details

The number of pathways in SBGNhub from each source database. It is calculated from data 'pathways.info'.

print.SBGNview *Generate image files*

Description

A wrapper to run function [renderSbgn](#) for all pathways in a SBGNview object and generate image files.

Usage

```
## S3 method for class 'SBGNview'  
print(x, ...)
```

Arguments

x A SBGNview class object.
... Other parameters passed to print.

Value

None

Examples

```
### Use simulated data. Please see vignettes for more examples.  
### Run `browseVignettes(package = "SBGNview")`  
data('pathways.info', 'sbgn.xmls')  
SBGNview.obj = SBGNview(simulate.data = TRUE,  
                          sbn.dir = './',  
                          input.sbn = 'P00001',  
                          output.file = './test.local.file',  
                          output.formats = c('pdf'),  
                          min.gene.value = -1,  
                          max.gene.value = 1)  
  
print(SBGNview.obj)
```

renderSbgn	<i>Overlay omics data on a SBGN pathway graph and output image files.</i>
------------	---

Description

This function is not intended to be used directly. Use SBGNview instead. Some input arguments can be better prepared by [SBGNview](#).

Usage

```
renderSbgn(  
  input.sbgn,  
  output.file,  
  output.formats,  
  sbgn.id.attr,  
  glyphs.user = list(),  
  arcs.user = list(),  
  arcs.info = "straight",  
  compartment.layer.info = "original",  
  user.data = matrix("no.user.data", nrow = 1),  
  if.plot.svg = TRUE,  
  key.pos = "topright",  
  color.panel.scale = 1,  
  color.panel.n.grid = 21,  
  col.gene.low = "green",  
  col.gene.high = "red",  
  col.gene.mid = "gray",  
  col.cpd.low = "blue",  
  col.cpd.high = "yellow",  
  col.cpd.mid = "gray",  
  min.gene.value = -1,  
  max.gene.value = 1,  
  mid.gene.value = 0,  
  min.cpd.value = -1,  
  max.cpd.value = 1,  
  mid.cpd.value = 0,  
  pathway.name = "",  
  pathway.name.font.size = 1,  
  if.plot.cardinality = FALSE,  
  multimer.margin = 5,  
  compartment.opacity = 1,  
  auxiliary.opacity = 1,  
  if.plot.annotation.nodes = FALSE,  
  inhibition.edge.end.shift = 5,  
  edge.tip.size = 6,  
  if.use.number.for.long.label = FALSE,  
  label.splitting.string = c(" ", ":", "-", ";", "/", "_"),
```

```

complex.compartment.label.margin = 8,
if.write.shorter.label.mapping = TRUE,
font.size = 3,
logic.node.font.scale = 3,
status.node.font.scale = 3,
node.width.adjust.factor = 2,
font.size.scale.gene = 3,
font.size.scale.cpd = 3,
font.size.scale.complex = 1.1,
font.size.scale.compartment = 1.6,
if.scale.complex.font.size = FALSE,
if.scale.compartment.font.size = FALSE,
node.width.adjust.factor.compartment = 0.02,
node.width.adjust.factor.complex = 0.02,
text.length.factor = 2,
text.length.factor.macromolecule = 2,
text.length.factor.compartment = 2,
text.length.factor.complex = 2,
space.between.color.panel.and.entity = 100,
global.parameters.list = NULL
)

```

Arguments

- `input.sbgn` A character string. The path to a local SBGN-ML file.
- `output.file`, `output.formats`, `sbgn.id.attr`
 These parameters are the same as the ones in [SBGNview](#). Please see [SBGNview](#) for more details.
- `glyphs.user` A list, optional. Each element is a 'glyph' object. The element names are glyph IDs (attribute 'id' of XHTML element 'glyph'). Note this is not affected by parameter 'sbgn.id.attr'. The glyph elements contain glyph meta-data for plotting (e.g. text size, border width, border color etc.). Please see the [glyph-class](#) documentation for more information. By default, SBGNview will run without this argument and return a glyph list extracted from the SBGN file. User can then customize this glyph list and assign it to 'glyphs.user' in the next SBGNview run to update the graph.
- `arcs.user` A list, optional. Each member is an 'arc' object. The element names are arc IDs (the value of 'id' attribute in XHTML element 'arc' or 'arc.spline' in the SBGN-ML file). Some SBGN-ML files have no arc IDs, in this case SBGNview will create an arc ID using 'source' and 'target' node IDs). The arc object contains arc meta-data for plotting (e.g. arc line width, line color etc.). Please see the [arc-class](#) documentation for more information. By default, SBGNview() will run without this argument and return an arc list. User can then customize this arc list and assign it to 'arcs.user' in the next SBGNview() run to update the arcs.
- `arcs.info` A character string. It should be one of the following: 'parse splines', 'straight' or a string of svg code of arcs. If it is 'parse splines', this function will look for XML element 'arc.spline' in the SBGN-ML file and plot spline arcs. If it is

'straight', the function will look for element 'arc' and plot straight line arcs. If it is a string of svg code, it will write this code directly to the output svg file.

<code>compartment.layer.info</code>	A character vector. It is a vector containing the IDs of all compartment glyphs. It determines the layer arrangement of compartments. Compartments will be drawn following their sequence in this vector. Therefore, a compartment that appears later in the vector will be on the front layer and covers the compartments that are before it in this vector. This is important. In some cases compartments have overlap. This layer information ensures that a glyph laying in the overlapped region belongs to the compartment on the top layer.
<code>user.data</code>	A list. It holds both gene/protein data and compound data. Names are gene or compounds, each element is a numeric vector of the omics data of each molecule.
<code>if.plot.svg</code>	Logical. Default: T. Whether to generate svg code or only parse SBGN-ML file. This parameter is for internal use only.
<code>key.pos</code>	A character string. The position of color panel. Default: 'topright'. Accepts one of 'bottomleft', 'bottomright', 'topright', or 'topleft'. The ideal position for the color panel is 'topright' or 'bottomright'. If 'topleft' or 'bottomleft' are passed in, the key.pos location will default to 'topright'. If key.pos is set to 'none', the pathway name and color panel won't be plotted.
<code>color.panel.scale</code>	Numeric. Default: 1. It controls the relative size of color scheme panel.
<code>color.panel.n.grid</code>	Numeric. Default: 21. How many colors does the color scheme show.
<code>col.gene.low</code>	A character string. Default: 'green'. Color panel's color representing low gene data values.
<code>col.gene.high</code>	A character string. Default: 'red'. Color panel's color representing high gene data values.
<code>col.gene.mid</code>	A character string. Default: 'gray'. Color panel's color representing mid range gene data values.
<code>col.cpd.low</code>	A character string. Default: 'blue'. Color panel's color representing low compound data values.
<code>col.cpd.high</code>	A character string. Default: 'yellow'. Color panel's color representing high compound data values.
<code>col.cpd.mid</code>	A character string. Default: 'gray'. Color panel's color representing mid range compound data values.
<code>min.gene.value</code>	Numeric. Default: -1. Color panel's min value for gene data. Values smaller than this will have the same color as min value.
<code>max.gene.value</code>	Numeric. Default: 1. Color panel's max value for gene data. Values greater than this will have the same color as the max value.
<code>mid.gene.value</code>	Numeric. Default: 0. Color panel's mid value for gene data.
<code>min.cpd.value</code>	Numeric. Default: -1. Color panel's min value for compound data. Values smaller than this will have the same color as min value.

<code>max.cpd.value</code>	Numeric. Default: 1. Color panel's max value for compound data. Values greater than this will have the same color as max value.
<code>mid.cpd.value</code>	Numeric. Default: 0. Color panel's mid value for compound data.
<code>pathway.name</code>	List containing two elements: 1. pathway name 2. stamp information. See argument description in SBGNview function to change/update pathway name displayed on graph.
<code>pathway.name.font.size</code>	Numeric. Default: 1. When pathway names are plotted on graph, this parameter controls their font size.
<code>if.plot.cardinality</code>	Logical. Default: F. If plot cardinality glyphs.
<code>multimer.margin</code>	Numeric. Default: 5. For multimers, they are represented by two partly overlapped shapes (rectangle, ellipse etc.). This parameter controls how much the two shapes overlap.
<code>compartment.opacity</code>	Numeric. Default: 1. Controls how transparent the compartments are.
<code>auxiliary.opacity</code>	Numeric. Default: 1. Controls opacity of auxiliary glyphs.
<code>if.plot.annotation.nodes</code>	Logical. Default: F. Some SBGN-ML files have 'annotation' glyphs. By default we don't plot them.
<code>inhibition.edge.end.shift</code>	Numeric. Default: 5. The tip of 'inhibition' arcs is a line segment. Sometimes it overlaps with target glyph's border. We can shift it along the arc to prevent the overlap.
<code>edge.tip.size</code>	Numeric. Default: 6. Control size of edge tips.
<code>if.use.number.for.long.label</code>	Logical. Default: F. If the label is too long, we can create a shorter name for it. e.g. 'macromolecule_1'.
<code>label.splitting.string</code>	A character vector. Default: <code>c(' ','-',';','/','_')</code> . When we split text into multiple lines, these characters will be used to split label (where a new line can be created).
<code>complex.compartment.label.margin</code>	Numeric. Default: 8. Move the label text vertically for compartment and complex.
<code>if.write.shorter.label.mapping</code>	Logical. Default: T. If <code>if.use.number.for.long.label</code> is 'T', we can write the mapping between shorter name and the original label to a text file.
<code>font.size</code>	Numeric. Default: 3. Affects font size of all types of glyphs.
<code>logic.node.font.scale</code>	Numeric. Default: 3. Controls the size of logical glyphs ('and', 'or', 'not' etc.).
<code>status.node.font.scale</code>	Numeric. Default: 3. Scale the font size for status variable and unit of information nodes.

- `node.width.adjust.factor`
Numeric. Default: 2. Change font size according to the width of its glyph. If the glyph is too large (e.g. compartment), its label may look too small. Then we can enlarge the label in proportion to the width of the glyph. It affects all types of glyphs.
- `font.size.scale.gene`
Numeric. Default: 3. Scales font size according to the node's width for large compartments. Only affect font size of 'macromolecule' glyphs.
- `font.size.scale.cpd`
Numeric. Default: 3. Scales font size according to the node's width for large compartments. Only affects font size of 'simple chemical' glyphs.
- `font.size.scale.complex`
Numeric. Default: 1.1. Scale the font size of a complex.
- `font.size.scale.compartment`
Numeric. Default: 1.6. Scale the font size of a compartment.
- `if.scale.complex.font.size`
Logical. Default: F. Whether to scale complex font size according to its width. If set to 'T', the 'node.width.adjust.factor.complex' argument can be used to specify the scale factor.
- `if.scale.compartment.font.size`
Logical. Default: F. Whether to scale compartment font size according to its width. If set to 'T', the 'node.width.adjust.factor.compartment' argument can be used to specify the scale factor.
- `node.width.adjust.factor.compartment`
Numeric. Default: 0.02. How much the font size should change in proportion to the width of compartment. The font is scaled only if 'if.scale.compartment.font.size' is set to 'T'. To find the best scale factor which works you, start with 0.02 (default) and incrementally increase that value.
- `node.width.adjust.factor.complex`
Numeric. Default: 0.02. How much the font size should change in proportion to the width of complex. The font is scaled only if 'if.scale.complex.font.size' is set to 'T'. To find the best scale factor which works you, start with 0.02 (default) and incrementally increase that value.
- `text.length.factor`
Numeric. Default: 2. How wide the wrapped text should be. If text is longer than the width controled by this parameter, the text is split into a new line, but only at characters in 'label.splitting.string'. Controls all glyphs.
- `text.length.factor.macromolecule`
Numeric. Default: 2. Used to determine label text wrapping based on number of characters, font size, and node width for macromolecule glyphs.
- `text.length.factor.compartment`
Numeric. Default: 2. Used to determine label text wrapping based on number of characters, font size, and node width for compartment glyphs.
- `text.length.factor.complex`
Numeric. Default: 2. Used to determine label text wrapping based on number of characters, font size, and node width for complex glyphs.

space.between.color.panel.and.entity

Numeric. Default: 100. The minimum space between color panel and any other object in the graph. The function will always try to find a location of the color panel to minimize empty space on the whole graph. This parameter controls how close it can reach a glyph.

global.parameters.list

List. A record of parameters fed to 'renderSbgn' for reuse. It will over-write other parameters. It is not designed to be used directly.

Value

A list of three elements: glyphs.list, arcs.list, global.parameters.list

Examples

```
## Not run:
data(pathways.info)
SBGNview.obj <- SBGNview(simulate.data = TRUE,
  sbgn.dir = './',
  input.sbgn = 'P00001',
  output.file = './test.local.file',
  output.formats = c('pdf'),
  min.gene.value = -1,
  max.gene.value = 1)

## End(Not run)
```

sbgn.gsets

Retrieve gene list or compound list from collected databases

Description

Retrieve gene list or compound list from collected databases

Usage

```
sbgn.gsets(
  id.type = "ENTREZID",
  mol.type = "gene",
  species = "hsa",
  database = "pathwayCommons",
  output.pathway.name = TRUE,
  combine.duplicated.set = TRUE,
  truncate.name.length = 50,
  SBGNview.data.folder = "./SBGNview.tmp.data"
)
```


Arguments

<code>id.type</code>	A character string. Default: "ENTREZID". The ID type of output gene list. One of the supported types in <code>data('mapped.ids')</code>
<code>mol.type</code>	A character string. Default: "gene". One of 'gene' or 'cpd'
<code>species</code>	A character string. Default: "hsa". The three letter species code used by KEGG. E.g. 'hsa', 'mmu'
<code>database</code>	A character string. Default: "pathwayCommons". The database where gene list will be extracted. Acceptable values: 'MetaCyc', 'pathwayCommons', 'MetaCROP'. The value is case in-sensitive.
<code>output.pathway.name</code>	Logical. Default: T. If set to 'TRUE', the names of returned list are in the format: 'pathway.id::pathway.name'. If set to 'FALSE', the format is 'pathway.id'
<code>combine.duplicated.set</code>	Logical. Default: T. Some pathways have the same geneset. If this parameter is set to 'TRUE', the output list will combine pathways that have the same gene set. The name in the list will be pathway names concatenated with ' '
<code>truncate.name.length</code>	Integer. Default: 50. The pathway names will be truncated to at most that length.
<code>SBGNview.data.folder</code>	A character string. Default: "./SBGNview.tmp.data". The path to a folder that will hold downloaded ID mapping files and pathway information data files.

Value

A list. Each element is a genelist of a pathway.

Examples

```
data(pathways.info)
mol.list <- sbgn.gsets(id.type = 'ENTREZID',
                      species = 'hsa',
                      database = 'pathwayCommons')
```

SBGNhub.id.mapping.tables

Mapping tables available in SBGNhub

Description

Mapping tables available in SBGNhub

Usage

```
data(SBGNhub.id.mapping.tables)
```

Format

A matrix

Details

A collection of ID mapping table files available in SBGNhub. If a matching mapping table is available, it will be downloaded from [SBGNhub](#) github page.

sbgnNodes

Extract glyph information

Description

This function will extract node information such as complex members, compartment members, node class, nodes with state variables etc.

Usage

```
sbgnNodes(  
  input.sbgn,  
  output.gene.id.type = NA,  
  output.cpd.id.type = NA,  
  database = NA,  
  species = NA,  
  show.ids.for.multiHit = NULL,  
  SBGNview.data.folder = "./SBGNview.tmp.data",  
  sbgn.dir = "./"  
)
```

Arguments

`input.sbgn` A character string. required. The pathway ID of pre-collected pathways or a path to a local SBGN-ML file.

`output.gene.id.type`
A character string. The desired output gene ID type. It only works when the SBGN-ML file is from one of these databases: 'MetaCyc' and 'pathway-Commons'. Currently, only 'macromolecule' glyphs are supported. Please check `data('mapped.ids')` for the types accepted. If omitted, the output IDs are the original IDs in the SBGN-ML file.

`output.cpd.id.type`
A character string. The desired output compound ID type. It only works when the SBGN-ML file is from one of these databases: 'MetaCyc' and 'pathway-Commons'. Currently, only 'simple chemical' glyphs are supported. Please check `data('mapped.ids')` for the types accepted. If omitted, the output IDs are the original IDs in the SBGN-ML file.

database	A character string. If the SBGN-ML file is from one of these databases: 'MetaCyc' and 'pathwayCommons', this parameter should be set to the corresponding string. For these two databases, this function can output other ID types instead of the original IDs in the SBGN-ML files. Otherwise, the output IDs are the original IDs in the 'id' attribute in the 'glyph' element.
species	A character string. Only output IDs from this particular species. It only works when the SBGN-ML file is from one of these databases: 'MetaCyc' and 'pathwayCommons'. Please check data('supported.species') for supported species. If omitted, the function will output IDs from all species.
show.ids.for.multiHit	Vector. When there are multiple output IDs mapped to a glyph, we only show the ones in this vector.
SBGNview.data.folder	A character string. Default: "./SBGNview.tmp.data". The path to a folder that will hold downloaded ID mapping files and pathway information data files.
sbgn.dir	A character string. Default: "./". The path to a folder that will hold created SBGN-ML files, if the input.sbgn are IDs of pre-collected pathways.

Details

The following glyph information is extracted: complex members, compartment members, submap members, node class, nodes with state variables, class of state variables, edges with cardinality, nodes with ports, 'source and sink' nodes, process nodes.

When trying to output other ID types, sometimes multiple output IDs are mapped to one glyph. In this situation, the IDs are concatenated by ';' to represent the glyph.

Value

A list containing extracted glyph information.

Examples

```
data(mapped.ids)
data(sbgn.xmls)
data(pathways.info)
node.list <- sbgnNodes(input.sbgn = 'P00001',
                      output.gene.id.type = 'ENTREZID',
                      output.cpd.id.type = 'compound.name',
                      species = 'hsa')
```

Description

This is the main function to map, integrate and render omics data on pathway graphs. Two inputs are needed: 1. A pathway file in SBGN-ML format and 2. gene and/or compound omics data. The function generates image file of a pathway graph with the omics data mapped to the glyphs and rendered as pseudo-colors. If no gene and/or compound omics data is supplied to the function, the function will output the SVG image file (and other selected file formats) of the parsed input file. This is useful for viewing the pathway graph without overlaid omics data. This function is similar to Pathview except the pathways are rendered with SBGN notation. In addition, users can control more graph properties including node/edge attributes. We collected SBGN-ML files from several pathway databases: Reactome, MetaCyc, MetaCrop, PANTHER and SMPDB. Given a vector of pathway IDs, SBGNview can automatically download and use these SBGN-ML files. To map omics data to glyphs, user just needs to specify omics data ID types. When using user customized SBGN-ML files, users need to provide a mapping file from omics data's molecule IDs to SBGN-ML file's glyph IDs.

Usage

```
SBGNview(
  gene.data = NULL,
  cpd.data = NULL,
  simulate.data = FALSE,
  input.sbgm = NULL,
  sbgn.dir = "./",
  output.file = "./output.svg",
  node.sum = "sum",
  gene.id.type = NA,
  cpd.id.type = NA,
  sbgn.id.attr = "id",
  sbgn.gene.id.type = NULL,
  sbgn.cpd.id.type = NA,
  id.mapping.gene = NULL,
  id.mapping.cpd = NULL,
  org = "hsa",
  output.formats = c("svg"),
  pathway.name = NULL,
  show.pathway.name = FALSE,
  SBGNview.data.folder = "./SBGNview.tmp.data",
  ...
)
```

Arguments

<code>gene.data</code>	A matrix, vector or SummarizedExperiment object. The same as 'gene.data' argument in package 'pathview', it is either a vector (single measurement) or a matrix-like data (multiple measurements). If the data is a vector, the entries should be numeric and names of entries should be gene IDs. Matrix data structure has genes as rows and samples as columns. Row names should be gene IDs.
------------------------	--

	Here gene ID is a generic concept, including multiple types: gene, transcript or protein. Default gene.data=NULL.
cpd.data	A matrix, vector or SummarizedExperiment object. The same as 'gene.data', except named with compound IDs. Default cpd.data=NULL.
simulate.data	Logical. SBGNview can simulate a dataset. If set to TRUE, SBGNview will simulate a gene data set and a compound dataset and user input 'gene.data' and 'cpd.data' are ignored.
input.sbn	A character vector. Can be either names of local SBGN files or pathway IDs of our pre-collected pathways. For pre-collected pathway IDs, run 'data(pathways.info)'
sbn.dir	A character string. Default: ".". The path to the folder that holds SBGN-ML files. If 'input.sbn' is a vector of pathway IDs in data 'pathways.info', the SBGN-ML files will be downloaded into this folder.
output.file	A character string. Default: "./output.svg". Path to the output image files. Because we often work with multiple pathways, each pathway will have its own image files. Each string in 'input.sbn' will be added to the end of 'output.file'. Depending on the image format specified by the 'output.formats' parameter, extensions will be added to the end (e.g. .pdf, .png etc.).
node.sum	A character string. Default: "sum". Sometimes multiple omics genes/compounds are mapped to one SBGN glyph. Therefore multiple values will be mapped to one measurement/slice on the glyph. In this situation, we may need to derive a single value for the slice on the glyph. This function can be any R function that takes a numeric vector as input and output a single numeric value (e.g. 'sum', 'max', 'min', 'mean'). It can also be a User Defined Function (UDF).
gene.id.type	A character string. The type of gene ID in 'gene.data'. This parameter is used for ID mapping. It should be one of the IDs in data 'mapped.ids'. For details, run: data('mapped.ids')
cpd.id.type	A character string. The type of compound ID in 'cpd.data'. For details, run: data('mapped.ids')
sbn.id.attr	A character string. This tells SBGNview where to find the ID of a glyph in SBGN-ML file for ID mapping. This ID is used to map omics data to the glyph. It is normally the name of an attribute in the 'glyph' element. For example: <glyph class='macromolecule' id='p53'> </glyph>. We can specify: sbn.id.attr = 'id'; sbn.gene.id.type = 'SYMBOL'. For our pre-generated SBGN-ML files , the ID attribute will be determined automatically thus can be omitted. Accepted values: 1. Any attribute name in element 'glyph' For example: <glyph class='macromolecule' id='p53' protein='P04637'> </glyph>. We can specify: sbn.id.attr = 'protein'; sbn.gene.id.type = 'UNIPROT', then 'P04637' will be the glyph ID. 2. The string 'label', this will make SBGNview use the glyph label as glyph ID. For example: <glyph id='glyph14' class='simple chemical'> <label text='L-alanine' /> </glyph>. We can specify: sbn.id.attr = 'label'; sbn.cpd.id.type = 'compound.name', then 'L-alanine' will be used as glyph ID.
sbn.gene.id.type	A character string. The ID type of "macromolecule" glyphs in SBGN-ML file (See parameter 'sbn.id.attr' for more details). This parameter is used for ID

mapping, i.e. either use our pre-generated mapping tables or find corresponding columns in user defined mapping tables in 'id.mapping.gene'. For **our pre-generated SBGN-ML files**, this will be determined automatically according to the pathway IDs thus can be omitted. For user defined SBGN-ML file, this parameter should be one of the column names of the matrix 'id.mapping.gene'.

sbgncpd.id.type	A character string. Similar to 'sbgngene.id.type'. The corresponding glyphs are "simple chemicals"
id.mapping.gene	A matrix. Mapping table between gene.id.type and sbgngene.id.type. This table is needed if the ID pair of gene.id.type and sbgngene.id.type is NOT included in data 'mapped.ids' or not mappable by package 'pathview'. This matrix should have two columns for gene.id.type and sbgngene.id.type, respectively. Column names should be the values of parameters 'sbgngene.id.type' and 'gene.id.type'. See example section for an example.
id.mapping.cpd	A matrix. See id.mapping.gene.
org	A character string. Default: "hsa". The species of the gene omics data. It is used for species specific gene ID mapping. Currently only supports three letters KEGG code (e.g. hsa, mmu, ath). For a complete list of KEGG codes, see this page: KEGG Organisms: Complete Genomes
output.formats	A character vector. It specifies the formats of output image files. The vector should be a subset of c('pdf', 'ps', 'png'). By default the function will always output a svg file. SBGNview uses rsvg to convert svg file to other formats. If other 'output.formats' is set but 'rsvg' package is not installed, an error will occur. See this page for how to install 'rsvg'
pathway.name	A character string. Change/update pathway name displayed on the output graph. If 'input.sbgncpd' is a pathway ID in data(pathways.info), the pathway name and database associated with the pathway ID will be displayed on the output graph. If 'input.sbgncpd' is a SBGN-ML file not part of our pre-generated SBGN-ML files, nothing will be displayed for the pathway name unless set using this argument.
show.pathway.name	Logical. Default: F. If set to TRUE and 'input.sbgncpd' are pre-collected pathway IDs, the pathway name will be added to the output file name.
SBGNview.data.folder	A character string. Default: "./SBGNview.tmp.data". The path to a folder that will hold temp data files.
...	Other parameters passed to function renderSbgncpd

Details

1. About SBGNview()

This function extracts glyph (node) and arc (edge) data from a SBGN-ML file and creates a SBGN graph from the extracted data (draws shapes etc. in SVG format). Then it maps omics data to the glyphs and renders data as colors. Currently it maps gene/protein omics data to 'macromolecule' glyphs and maps compound omics data to 'simple chemical' glyphs.

2. About SBGN-ML files and curved arcs encoding

SBGNview can parse SBGN-ML files with standard SBGN PD syntax. For arcs, SBGNview can handle both straight lines (standard SBGN PD syntax) and spline curves (a syntax add by us). Current SBGN-ML syntax supports straight lines. The coordinates of line start or end points are stored in element 'arc'. But straight lines often produce node-edge or edge-edge crossings. Therefore, we generated SBGN-ML files with pre-routed spline edges.

To store the routed splines, we added an XHTML element called 'edge.spline.info', which has children elements called 'arc.spline'. Each 'arc.spline' element has three types of children elements: 'source.arc', 'target.arc' and 'spline'. 'source.arc' and 'target.arc' will be rendered as straight line arcs controlled by attributes 'start.x', 'start.y', 'end.x', 'end.y' (line ends' coordinates) and 'class' (type of the straight line arc). These two arcs ensure the notation of the spline arc comply with its class. 'spline' will be rendered as splines connecting 'source.arc' and 'target.arc'. Each 'spline' is defined by coordinates of four points: s (starting point of spline), c1 (the first control point of spline), c2 (the second control point of spline) and e (ending point of spline). In case of complicated routing, there could be multiple 'splines' in an 'arc.spline'.

The function first checks if the SBGN-ML file has spline arcs (XHTML element 'edge.spline.info') and use it if found. When there are no spline arcs, it will use straight line arcs (XHTML element 'arc'). Please check out examples in [our SBGN-ML file collection](#).

3. About ID mapping

SBGNview can automatically map several ID types to glyphs of pathwayCommons, MetaCyc and MetaCrop. For user defined SBGN-ML file, users need to provide information about how to map their omics data to glyphs.

3.1 How SBGNview finds glyph IDs in SBGN-ML file: Glyph IDs are recorded in attribute 'id' in XHTML element 'glyph'. But for ID mapping, user can use other attributes by changing parameter 'sbn.id.attr'.

3.2 For [our SBGN-ML file collection](#)., SBGNview can do ID mapping automatically. It uses extracted mapping between 1) UNIPROT/uniref and 'macromolecule' glyph IDs and 2) ChEBI and 'simple chemical' glyph IDs from biopax files in pathwayCommons and MetaCyc. For other ID types, we used pathview (gene/protein) and UniChem (compound) to map to UNIPROT and ChEBI, respectively, then map them to glyph IDs. For MetaCrop, we used pathview for ID mapping.

4. Two common scenarios of using SBGNview

4.1 Using [our pre-generated SBGN-ML files](#).

Supported pathways can be found using data('pathways.info'). This is a collection of SBGN-ML files for these databases: MetaCyc, MetaCrop and three databases collected by pathwayCommons (PANTHER Pathway, Reactome and SMPDB). For SBGN-ML each file, the glyph layout is based on fdp and optimized to eliminate glyph-glyph overlaps. The arcs are splines that are routed to eliminate arc-glyph crossings.

To use these data, SBGNview needs the following parameters:

-gene.id.type and/or cpd.id.type (at least one should be provided)

SBGNview can map omics data to SBGN-ML glyphs automatically. Supported ID types can be found in data('mapped.ids')

Input SBGN-ML files can be obtained by using function 'downloadSbnFile'.

4.2 Using SBGN-ML files from other sources.

4.2.1 Input omics data have the SAME ID type as the glyph ID type in SBGN-ML file:

In this scenario, SBGNview needs the following information to map omics data to SBGN-ML glyphs:

-ID type of input omics data (gene.id.type and/or cpd.id.type)

-ID type of glyphs of input SBGN-ML file (sbn.gene.id.type and/or sbgn.cpd.id.type).

These ID types can be any characters, but gene.id.type must be the same as sbgn.gene.id.type, and cpd.id.type must be the same as sbgn.cpd.id.type.

Users can use the function 'changeDataId' to change the omics IDs to the glyph IDs in SBGN-ML file.

4.2.2 Input omics data have DIFFERENT ID type as the glyph ID type in SBGN-ML file:

In this scenario, SBGNview needs the following information to map omics data to SBGN-ML glyphs:

-ID type of input omics data (gene.id.type and/or cpd.id.type)

-ID type of glyphs of input SBGN-ML file (sbn.gene.id.type and/or sbgn.cpd.id.type).

-A mapping table between input omics IDs and SBGN-ML glyph IDs (id.mapping.gene and/or id.mapping.cpd).

For user's convenience, pathview can generate such tables for several ID types (functions 'geneannot.map' and 'cpdidmap'). But column names need to be changed to the values of 'gene.id.type' and 'sbn.gene.id.type'.

Value

SBGNview object (S3 class object) which is a list containing three elements:

1. data:
2. output.file: A string of the path to the output file. It is the string set by parameter 'output.file' in function SBGNview.
3. output.formats: A character vector specifying the formats of output image files. The vector should be a subset of c('pdf', 'ps', 'png'). By default the function will always output a svg file.

This S3 class of objects contains information generated by the SBGNview function. The SBGNview object can be modified by using the "+" binary operator in conjunction with the [highlightArcs](#), [highlightNodes](#), and [highlightPath](#) functions. This mechanism to allow layer-by-layer graph modification is similar to that of ggplot2, a widely used R package for data visualization. Defining this class as a formal (S4) class will produce an S4 SBGNview object which doesn't work with the binary operator and doesn't allow for layer-by-layer graph modification. Therefore, we decided to go with the S3 implementation of the SBGNview class since it works well with the binary operator making this functionality more intuitive and user friendly.

Examples

```
### Use simulated data. Please see vignettes for more examples.
### Run `browseVignettes(package = "SBGNview")`

# load demo dataset, SBGN pathway data collection and info, which may take a few seconds
# we use a cancer microarray dataset 'gse16837.d' from package 'pathview'
data("gse16873.d", "pathways.info", "sbn.xmls")
```



```
# search for pathways with user defined keywords
input.pathways <- findPathways("Adrenaline and noradrenaline biosynthesis")

# render SBGN pathway graph and output image files
SBGNview.obj <- SBGNview(gene.data = gse16873.d[,1:3],
  gene.id.type = "entrez",
  input.sbgm = input.pathways$pathway.id,
  output.file = "quick.start",
  output.formats = c("png", "pdf"),
  min.gene.value = -1,
  max.gene.value = 1)

SBGNview.obj
```

spline.arc-class

An object to store information of spline arcs

Description

An object to store information of spline arcs

Details

Arc information comes from two sources: 1. SBGN-ML file's 'arc' element ('source', 'target', coordinates etc.). 2. Parameters specified when running [SBGNview](#). User can modify arc objects to change the way how they are rendered. See the "arcs.user" argument in [renderSbgm](#).

Slots

target, source, id, arc.class A character string. Information extracted from element 'arc.spline'.

start.x, start.y, end.x, end.y Numeric. Information extracted from elements 'start', 'end' or 'next'.

stroke.opacity Numeric. Controls the line of an arc (not tip of arc).

components A list of 'arc' and 'spline' objects. A spline arc is represented by several components: 1. The two ends of the arc are represented by straight line 'arc' objects. 2. splines connecting the ends are represented by 'spline' objects.

parameters.list A list. The parameters.list slot is a copy of the global.parameters.list. The global.parameters.list contains the '...' parameters passed into [SBGNview](#) which will be used by [renderSbgm](#). By default this slot for all spline.arc objects in the output SBGNview object will be an empty list. You can add named elements to this slot to customize each individual spline.arc. For information about which parameters can be set in the parameters.list slot, see the arguments in [renderSbgm](#). A customized list of arc objects can be passed as input into SBGNview function using the 'arcs.user' argument (see [renderSbgm](#) for more information).

edge A list. An arc in SBGN map normally consists of a line and a tip shape at the end of the line. This list holds variables that controls arc properties. Available elements can be accessed as follow:

The following three parameters control the line:

arc@edge\$line.stroke.color
arc@edge\$line.stroke.opacity
arc@edge\$line.width

The following five parameters control the tip:

arc@edge\$tip.stroke.opacity
arc@edge\$tip.stroke.color
arc@edge\$tip.stroke.width
arc@edge\$tip.fill.color
arc@edge\$tip.fill.opacity

Index

- * **datasets**
 - mapped.ids, [15](#)
 - pathways.info, [17](#)
 - pathways.stats, [17](#)
 - SBGNhub.id.mapping.tables, [25](#)
- + .SBGNview, [3](#)
- arc-class, [3](#)
- changeDataId, [4](#), [6](#)
- changeIds, [4](#), [6](#)
- downloadSbgnFile, [7](#)
- findPathways, [8](#)
- glyph-class, [9](#)
- highlightArcs, [10](#), [32](#)
- highlightNodes, [3](#), [11](#), [32](#)
- highlightPath, [3](#), [12](#), [32](#)
- loadMappingTable, [14](#)
- mapped.ids, [15](#)
- outputFile, [16](#)
- outputFile<-, [16](#)
- pathways.info, [17](#)
- pathways.stats, [17](#)
- print.SBGNview, [18](#)
- renderSbgn, [3](#), [4](#), [9](#), [10](#), [18](#), [19](#), [30](#), [33](#)
- sbgn.gsets, [24](#)
- SBGNhub.id.mapping.tables, [25](#)
- sbgnNodes, [26](#)
- SBGNview, [3](#), [4](#), [10](#), [19](#), [20](#), [22](#), [27](#), [33](#)
- spline.arc-class, [33](#)