

# Package ‘ROntoTools’

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**Type** Package

**Title** R Onto-Tools suite

**Version** 1.6.1

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**Description** Suite of tools for functional analysis

**biocViews** NetworkAnalysis, Microarray, GraphsAndNetworks

**License** GPL (>= 3)

**Depends** methods, graph, boot, KEGGREST, KEGGgraph, Rgraphviz

**Suggests** RUnit, BiocGenerics

**Collate** 'pathwayExpress.R' 'utils.R' 'graphWeights.R' 'keggDataREST.R'  
'AllClasses.R' 'AllGenerics.R' 'nodeWeights-methods.R'  
'pePathway-utils.R' 'Summary-methods.R' 'plot-methods.R'  
'renderInfo-methods.R'

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---

alpha1MR	<i>Compute alpha weights</i>
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---

**Description**

Transform a vector of p-values into weights.

**Usage**

```
alpha1MR(pv, threshold = max(pv))
```

**Arguments**

pv	vector of p-values
threshold	the threshold value that was used to select DE genes

**Details**

Computes a set of weights from p-values using the formula  $1-pv/threshold$ .

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[pe](#)

**Examples**

```
load(system.file("extdata/E-GEOD-21942.topTable.RData", package = "ROntoTools"))  
head(alpha1MR(top$adj.P.Val))
```

---

alphaMLG	<i>Compute alpha weights</i>
----------	------------------------------

---

**Description**

Transform a vector of p-values into weights.

**Usage**

```
alphaMLG(pv, threshold = max(pv))
```

**Arguments**

pv	vector of p-values
threshold	the threshold value that was used to select DE genes

**Details**

Computes a set of weights from p-values using the formula  $-\log_{10}(pv/threshold)$ .

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[pe](#)

**Examples**

```
load(system.file("extdata/E-GEOD-21942.topTable.RData", package = "ROntoTools"))
head(alphaMLG(top$adj.P.Val))
```

---

compute.fisher	<i>Combine independent p-values using the Fisher method</i>
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---

**Description**

Combine independent p-values using the Fisher method

**Usage**

```
compute.fisher(p, eps = 1e-06)
```

**Arguments**

p a vector of independent p-values  
eps the minimal p-value considered (all p-values smaller will be set to this value)

**Author(s)**

Calin Voichita and Sorin Draghici

**References**

Tarca AL., Draghici S., Khatri P., Hassan SS., Kim J., Kim CJ., Kusanovic JP., Romero R.: "A Signaling Pathway Impact Analysis for Microarray Experiments", 2008, Bioinformatics, 2009, 25(1):75-82.

**See Also**

[pe,compute.normalInv](#)

**Examples**

```
p <- c(.1, .01)
compute.fisher(p)
```

---

compute.normalInv *Combine independent p-values using the normal inversion method*

---

**Description**

Combine independent p-values using the normal inversion method

**Usage**

```
compute.normalInv(p, eps = 1e-06)
```

**Arguments**

p a vector of independent p-values  
eps the minimal p-value considered (all p-values smaller will be set to this value)

**Author(s)**

Calin Voichita and Sorin Draghici

**References**

Tarca AL., Draghici S., Romero R.: "A Mmore Specific Method To Combine Perturbation and Over-representation Evidence in Pathway Analysis", PSB 2010 poster.

**See Also**

[pe,compute.fisher](#)

**Examples**

```
p <- c(.1, .01)
compute.normalInv(p)
```

---

keggPathwayGraphs      *Download and parse KEGG pathway data*

---

**Description**

Download and parse KEGG pathway data

**Usage**

```
keggPathwayGraphs(organism = "hsa",
  targRelTypes = c("GErel", "PCrel", "PPrel"),
  relPercThresh = 0.9, nodeOnlyGraphs = FALSE,
  updateCache = FALSE, verbose = TRUE)
```

**Arguments**

organism	organism code as defined by KEGG
targRelTypes	target relation types
relPercThresh	percentage of the number of relation types over all possible realtions in the pathway
nodeOnlyGraphs	allow graphs with no edges
updateCache	re-download KEGG data
verbose	show progress of downloading and parsing

**Value**

A list of [graphNEL](#) objects encoding the pathway information.

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[keggPathwayNames](#)

**Examples**

```
# The pathway cache provided as part of the pathway contains only the
# pathways that passed the default filtering. We recommend, re-downloading
# the pathways using the updateCache parameter
kpg <- keggPathwayGraphs("hsa")

# to update the pathway cache for human run:
# kpg <- keggPathwayGraphs("hsa", updateCache = TRUE)
# this is time consuming and depends on the available bandwidth.

head(names(kpg))

kpg[["path:hsa04110"]]
head(nodes(kpg[["path:hsa04110"]]))
head(edges(kpg[["path:hsa04110"]]))
```

---

keggPathwayNames	<i>Obtain KEGG pathway titles</i>
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---

**Description**

Obtain KEGG pathway titles

**Usage**

```
keggPathwayNames(organism = "hsa", updateCache = FALSE,
  verbose = TRUE)
```

**Arguments**

organism	organism code as defined by KEGG
updateCache	re-download KEGG data
verbose	show progress of downloading and parsing

**Value**

A named vector of pathway titles. The names of the vector are the pathway KEGG IDs.

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[keggPathwayGraphs](#)

## Examples

```
kpn <- keggPathwayNames("hsa")

# to update the pathway cache for human run:
# kpn <- keggPathwayNames("hsa", updateCache = TRUE)
# this is time consuming and depends on the available bandwidth.

head(kpn)
```

---

nodeWeights

*Retrieve the node weights of a graph*

---

## Description

A generic function that returns the node weights of a graph. If `index` is specified, only the weights of the specified nodes are returned. The user can control which node attribute is interpreted as the weight.

## Arguments

<code>object</code>	A graph, any object that inherits the graph class.
<code>index</code>	If supplied, a character or numeric vector of node names or indices.
<code>...</code>	Unused.
<code>attr</code>	The name of the node attribute to use as a weight. You can view the list of defined node attributes and their default values using <code>nodeDataDefaults</code> .
<code>default</code>	The value to use if <code>object</code> has no node attribute named by the value of <code>attr</code> . The default is the value 1.

## Details

The weights of all nodes identified by the `index` are returned. If `index` is not supplied, the weights of all nodes are returned.

By default, `nodeWeights` looks for an node attribute with name "weight" and, if found, uses these values to construct the node weight vector. You can make use of attributes stored under a different name by providing a value for the `attr` argument. For example, if `object` is a graph instance with an node attribute named "WTS", then the call `nodeWeights(object, attr="WTS")` will attempt to use those values.

If the graph instance does not have an node attribute with name given by the value of the `attr` argument, `default` will be used as the weight for all nodes. Note that if there is an attribute named by `attr`, then its default value will be used for nodes not specifically customized. See `nodeData` and `nodeDataDefaults` for more information.

## Value

A named vector with the node weights. The names of the vector are the names of the specified `index`, or all nodes if `index` was not provided.

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[nodes](#), [nodeData](#)

**Examples**

```
library(graph)
V <- LETTERS[1:4]
g <- graphNEL(nodes = V, edgemode = "directed")
nodeWeights(g)
nodeWeights(g, "B")
nodeWeights(g, attr = "WT", default = 3)
```

---

pe

*Pathway-Express: Pathway analysis of signaling pathways*

---

**Description**

Pathway-Express: Pathway analysis of signaling pathways

**Usage**

```
pe(x, graphs, ref = NULL, nboot = 2000, verbose = TRUE,
   cluster = NULL, seed = NULL)
```

**Arguments**

x	named vector of log fold changes for the differentially expressed genes; names(x) must use the same id's as ref and the nodes of the graphs
graphs	list of pathway graphs as objects of type graph (e.g., <a href="#">graphNEL</a> ); the graphs must be weighted graphs (i.e., have an attribute weight for both nodes and edges)
ref	the reference vector for all genes in the analysis; if the reference is not provided or it is identical to names(x) a cut-off free analysis is performed
nboot	number of bootstrap iterations
verbose	print progress output
cluster	a cluster object created by <a href="#">makeCluster</a> for parallel computations
seed	an integer value passed to <a href="#">set.seed()</a> during the bootstrap permutations

**Details**

See details in the cited articles.

**Value**

An object of class [peRes](#).

**Author(s)**

Calin Voichita and Sorin Draghici

**References**

Voichita C., Donato M., Draghici S.: "Incorporating gene significance in the impact analysis of signaling pathways", IEEE Machine Learning and Applications (ICMLA), 2012 11th International Conference on, Vol. 1, p.126-131, 2012

Tarca AL., Draghici S., Khatri P., Hassan SS., Kim J., Kim CJ., Kusanovic JP., Romero R.: "A Signaling Pathway Impact Analysis for Microarray Experiments", 2008, Bioinformatics, 2009, 25(1):75-82.

Khatri P., Draghici S., Tarca AL., Hassan SS., Romero R.: "A system biology approach for the steady-state analysis of gene signaling networks". Progress in Pattern Recognition, Image Analysis and Applications, Lecture Notes in Computer Science. 4756:32-41, November 2007.

Draghici S., Khatri P., Tarca A.L., Amin K., Done A., Voichita C., Georgescu C., Romero R.: "A systems biology approach for pathway level analysis". Genome Research, 17, 2007.

**See Also**

[Summary](#), [plot.peRes](#), [keggPathwayGraphs](#), [setNodeWeights](#), [setEdgeWeights](#)

**Examples**

```
# load a multiple sclerosis study (public data available in Array Express
# ID: E-GEOD-21942)
# This file contains the top table, produced by the limma package with
# added gene information. All the probe sets with no gene associate to them,
# have been removed. Only the most significant probe set for each gene has been
# kept (the table is already ordered by p-value)
# The table contains the expression fold change and significance of each
# probe set in peripheral blood mononuclear cells (PBMC) from 12 MS patients
# and 15 controls.
load(system.file("extdata/E-GEOD-21942.topTable.RData", package = "ROntoTools"))
head(top)

# select differentially expressed genes at 1% and save their fold change in a
# vector fc and their p-values in a vector pv
fc <- top$logFC[top$adj.P.Val <= .01]
names(fc) <- top$entrez[top$adj.P.Val <= .01]

pv <- top$P.Value[top$adj.P.Val <= .01]
names(pv) <- top$entrez[top$adj.P.Val <= .01]

# alternatively use all the genes for the analysis
# NOT RUN:
# fc <- top$logFC
```

```

# names(fc) <- top$entrez

# pv <- top$P.Value
# names(pv) <- top$entrez

# get the reference
ref <- top$entrez

# load the set of pathways
kpg <- keggPathwayGraphs("hsa")

# set the beta information (see the cited documents for meaning of beta)
kpg <- setEdgeWeights(kpg)

# include the significance information in the analysis (see Voichita:2012
# for more information)
# set the alpha information based on the pv with one of the predefined methods
kpg <- setNodeWeights(kpg, weights = alphaMLG(pv), defaultWeight = 1)

# perform the pathway analysis
# in order to obtain accurate results the number of bootstraps, nboot, should
# be increase to a number like 2000
peRes <- pe(fc, graphs = kpg, ref = ref, nboot = 100, verbose = TRUE)

# obtain summary of results
head(Summary(peRes))

```

---

peEdgeRenderInfo

*Extract edge render information from a pePathway object*


---

## Description

Extract edge render information from a pePathway object

## Usage

```

peEdgeRenderInfo(x, pos.col = "black", pos.lty = "solid",
  pos.ah = "vee", neg.col = "black", neg.lty = "dashed",
  neg.ah = "tee", zero.col = "lightgray",
  zero.lty = "dotted", zero.ah = "none")

```

## Arguments

x	an object of class <a href="#">pePathway</a>
pos.col	color of the edges with possitive weight
pos.lty	line type of the edges with possitive weight
pos.ah	arrow head of the edges with possitive weight
neg.col	color of the edges with negative weight

neg.lty	line type of the edges with negative weight
neg.ah	arrow head of the edges with negative weight
zero.col	color of the edges with zero weight
zero.lty	color of the edges with zero weight
zero.ah	color of the edges with zero weight

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[edgeRenderInfo,par](#)

**Examples**

```
# load experiment
load(system.file("extdata/E-GEOD-21942.topTable.RData", package = "ROntoTools"))
fc <- top$logFC[top$adj.P.Val <= .01]
names(fc) <- top$entrez[top$adj.P.Val <= .01]
ref <- top$entrez

# load the set of pathways
kpg <- keggPathwayGraphs("hsa")
kpg <- setEdgeWeights(kpg)
kpg <- setNodeWeights(kpg, defaultWeight = 1)

# perform the pathway analysis
peRes <- pe(fc, graphs = kpg, ref = ref, nboot = 100, verbose = TRUE)

p <- peRes@pathways[[50]]
g <- layoutGraph(p@map, layoutType = "dot")
graphRenderInfo(g) <- list(fixedsize = FALSE)
edgeRenderInfo(g) <- peEdgeRenderInfo(p)
nodeRenderInfo(g) <- peNodeRenderInfo(p)
# notice the different type of edges in the graph (solid/dashed/dotted)
renderGraph(g)
```

---

peNodeRenderInfo

*Extract node render information from a pePathway object*

---

**Description**

Extract node render information from a pePathway object

**Usage**

```
peNodeRenderInfo(x, y = "Pert", input.shape = "box",
  default.shape = "ellipse", pos.col = "red",
  neg.col = "blue", zero.col = "white")
```

**Arguments**

x	an object of class <a href="#">pePathway</a>
y	a string representing the factor to be represented (Pert, Acc or input; see <a href="#">pePathway</a> )
input.shape	shape of nodes that have measured expression change
default.shape	shape of all other nodes
pos.col	color of nodes with a positive y factor
neg.col	color of nodes with a negative y factor
zero.col	color of nodes with the y factor equal to zero

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[nodeRenderInfo,par](#)

**Examples**

```
# load experiment
load(system.file("extdata/E-GEOD-21942.topTable.RData", package = "ROntoTools"))
fc <- top$logFC[top$adj.P.Val <= .01]
names(fc) <- top$entrez[top$adj.P.Val <= .01]
ref <- top$entrez

# load the set of pathways
kpg <- keggPathwayGraphs("hsa")
kpg <- setEdgeWeights(kpg)
kpg <- setNodeWeights(kpg, defaultWeight = 1)

# perform the pathway analysis
peRes <- pe(fc, graphs = kpg, ref = ref, nboot = 100, verbose = TRUE)

p <- peRes@pathways[[50]]
g <- layoutGraph(p@map, layoutType = "dot")
graphRenderInfo(g) <- list(fixedsize = FALSE)
edgeRenderInfo(g) <- peEdgeRenderInfo(p)
nodeRenderInfo(g) <- peNodeRenderInfo(p)
# notice the different type of nodes in the graph (box/circle)
# the color of each node represents the perturbation (red = positive, blue = negative)
# the shade represents the strength of the perturbation
renderGraph(g)
```

```
nodeRenderInfo(g) <- peNodeRenderInfo(p, "Acc")  
# now, the color of each node represents the accumulation (red = positive, blue = negative)  
# notice that square nodes with no parents have no accumulation  
renderGraph(g)
```

---

pePathway	<i>Class that encodes the result of Pathway-Express for a single pathway</i>
-----------	--

---

### Description

Class that encodes the result of Pathway-Express for a single pathway

### Slots

**map:** an object of type graph (e.g., [graphNEL](#)).  
**input:** named vector of fold changes for genes on this pathway. The names of the genes are the original IDs used in the analysis  
**ref:** vector of reference IDs on this pathway  
**boot:** an object of class boot encoding the bootstrap information.  
**Pert:** the gene perturbation factors for all genes on the pathway, as computed by Pathway-Express.  
**Acc:** the gene accumulations for all genes on the pathway, as computed by Pathway-Express.

### Author(s)

Calin Voichita and Sorin Draghici

### See Also

[pe](#), [peRes](#)

---

peRes	<i>Pathway-Express result class</i>
-------	-------------------------------------

---

### Description

This class is used to encode the results of the pathway analysis performed by the function [pe](#).

### Details

The slots `input` and `ref` record global information related to the whole analysis, while the `pathways` slot records the specific results as [pePathway](#) for each one of the pathways used in the analysis.

**Slots**

pathways: A list of [pePathway](#) objects.

input: named vector of fold changes used for the analysis. The names of the vector are the IDs originally used.

ref: character vector containing the IDs used as reference in the analysis.

cutOffFree: boolean value indicating if a cut-of-free analysis has been performed.

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[pe](#), [pePathway](#)

---

plot.pePathway

*Plot pathway level statistics*

---

**Description**

Display graphical representation of pathway level statistic like: i) two way comparison between the measured expression change and one of the factors computed by Pathway-Express ([pe](#)) or ii) the bootstrap statistics of the same factors.

**Arguments**

x	an object of type <a href="#">pePathway</a>
y	if provided, the factor to be plotted (either Acc (default) or Pert; see <a href="#">pePathway</a> )
...	Arguments to be passed to methods, such as <a href="#">par</a>
type	type of plot (either two.way (default) or boot)
eps	any value smaller than this will be plotted as 0

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[pe](#), [plot.peRes](#), [peNodeRenderInfo](#), [peEdgeRenderInfo](#)

**Examples**

```

# load experiment
load(system.file("extdata/E-GEOD-21942.topTable.RData", package = "ROntoTools"))
fc <- top$logFC[top$adj.P.Val <= .01]
names(fc) <- top$entrez[top$adj.P.Val <= .01]
ref <- top$entrez

# load the set of pathways
kpg <- keggPathwayGraphs("hsa")
kpg <- setEdgeWeights(kpg)
kpg <- setNodeWeights(kpg, defaultWeight = 1)

# perform the pathway analysis (for more accurate results use nboot = 2000)
peRes <- pe(fc, graphs = kpg, ref = ref, nboot = 100, verbose = TRUE)

plot(peRes@pathways[[50]])

plot(peRes@pathways[[50]], "Pert", main = "Perturbation factor")

plot(peRes@pathways[[50]], type = "boot")

plot(peRes@pathways[[50]], "Pert", type = "boot", main = "Perturbation factor")

```

---

plot.peRes

*Plot Pathway-Express result*


---

**Description**

Display a two-way plot using two of the p-values from the Pathway-Express analysis.

**Arguments**

x	an object of type <a href="#">peRes</a>
y	vector of two p-values names to be combined using <code>comb.pv.func</code> (default: <code>c("pAcc", "pORA")</code> ).
...	Arguments to be passed to methods, such as <a href="#">par</a> .
<code>comb.pv.func</code>	the function to combine the p-values - takes as input a vector of p-values and returns the combined p-value (default: <a href="#">compute.fisher</a> ).
<code>adjust.method</code>	the name of the method to adjust the p-value (see <a href="#">p.adjust</a> )
<code>threshold</code>	corrected p-value threshold
<code>eps</code>	any value smaller than this will be considered as eps (default: 1e-6).

**Author(s)**

Calin Voichita and Sorin Draghici

**See Also**

[pe](#), [Summary.peRes](#), [plot.pePathway](#)

**Examples**

```
# load experiment
load(system.file("extdata/E-GEO-21942.topTable.RData", package = "ROntoTools"))
fc <- top$logFC[top$adj.P.Val <= .01]
names(fc) <- top$entrez[top$adj.P.Val <= .01]
ref <- top$entrez

# load the set of pathways
kpg <- keggPathwayGraphs("hsa")
kpg <- setEdgeWeights(kpg)
kpg <- setNodeWeights(kpg, defaultWeight = 1)

# perform the pathway analysis (for more accurate results use nboot = 2000)
peRes <- pe(fc, graphs = kpg, ref = ref, nboot = 100, verbose = TRUE)

plot(peRes)

plot(peRes, c("pPert", "pORA"), comb.pv.func = compute.normalInv, threshold = .01)
```

---

setEdgeWeights	<i>Set gene weights based on edge type</i>
----------------	--

---

**Description**

setEdgeWeights

**Usage**

```
setEdgeWeights(graphList, edgeTypeAttr = "subtype",
  edgeWeightByType = list(activation = 1, inhibition = -1, expression = 1, repression = -1),
  defaultWeight = 0, combineWeights = sum,
  nodeOnlyGraphs = FALSE)
```

**Arguments**

graphList	a list of <a href="#">graphNEL</a> objects
edgeTypeAttr	edge attribute to be considered as the edge type. If the edge has multiple types, the edge type attribute is considered as a comma separated list of types
edgeWeightByType	named list of weights, where the names of the list are the edge type (values of the attribute defined by edgeTypeAttr)
defaultWeight	default value for an edge with a type not defined in edgeWeightByType

- combineWeights for the edges with multiple types, the function to be applied on the vector of weights
- nodeOnlyGraphs boolean value marking if graphs with no edges should be returned or not; note that graphs with all edge weights equal to 0 are considered node only graphs

**Value**

The graphList with the edge weights set.

**Author(s)**

Calin Voichita and Sorin Draghici

**Examples**

```
# load the set of pathways
kpg <- keggPathwayGraphs("hsa")

kpg <- setEdgeWeights(kpg)

edgeWeights(kpg[["path:hsa04110"]])
```

---

setNodeWeights      *Set node weights*

---

**Description**

Set node weights

**Usage**

```
setNodeWeights(graphList, weights = NULL,
               defaultWeight = 1)
```

**Arguments**

- graphList a list of graph (e.g., [graphNEL](#)) objects
- weights named vector or matrix; if vector, the node is going to have the same weight in all graphs it appears; if matrix, the rows represent nodes and columns represent graphs and the node will have different weights in each pathway
- defaultWeight the default weight for all nodes not set by the parameter weights

**Value**

The graphList with the node weights set.

**Author(s)**

Calin Voichita and Sorin Draghici

**Examples**

```
# load the set of pathways
kpg <- keggPathwayGraphs("hsa")

kpg <- setNodeWeights(kpg)

nodeWeights(kpg[["path:hsa04110"]])
```

---

Summary

*Summarize the results of a Pathway-Express analysis*

---

**Description**

Summarize the results of a Pathway-Express analysis

**Arguments**

x	Pathways-Express result object obtained using <a href="#">pe</a>
pathNames	named vector of pathway names; the names of the vector are the IDs of the pathways
totalAcc	boolean value indicating if the total accumulation should be computed
totalPert	boolean value indicating if the total perturbation should be computed
normalize	boolean value indicating if normalization with regards to the bootstrap simulations should be performed on totalAcc and totalPert
pPert	boolean value indicating if the significance of the total perturbation in regards to the bootstrap permutations should be computed
pAcc	boolean value indicating if the significance of the total accumulation in regards to the bootstrap permutations should be computed
pORA	boolean value indicating if the over-representation p-value should be computed
comb.pv	vector of the p-value names to be combine (any of the above p-values)
comb.pv.func	the function to combine the p-values; takes as input a vector of p-values and returns the combined p-value
order.by	the name of the p-value that is used to order the results
adjust.method	the name of the method to adjust the p-value (see <a href="#">p.adjust</a> )

**See Also**

[pe](#)

**Examples**

```
# load experiment
load(system.file("extdata/E-GEOD-21942.topTable.RData", package = "ROntoTools"))
fc <- top$logFC[top$adj.P.Val <= .01]
names(fc) <- top$entrez[top$adj.P.Val <= .01]
ref <- top$entrez

# load the set of pathways
kpg <- keggPathwayGraphs("hsa")
kpg <- setEdgeWeights(kpg)
kpg <- setNodeWeights(kpg, defaultWeight = 1)

# perform the pathway analysis
peRes <- pe(fc, graphs = kpg, ref = ref, nboot = 100, verbose = TRUE)

# obtain summary of results
head(Summary(peRes))

kpn <- keggPathwayNames("hsa")

head(Summary(peRes))

head(Summary(peRes, pathNames = kpn, totalAcc = FALSE, totalPert = FALSE,
             pAcc = FALSE, pORA = FALSE, comb.pv = NULL, order.by = "pPert"))
```

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