Package 'g2f'

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Type Package

Title Find and Fill Gaps in Metabolic Networks

Version 0.2

Description For a given metabolic network, this package finds the gaps (metabolites not produced or not consumed in any other reaction), and fills it from the stoichiometric reactions of a reference metabolic reconstruction using a weighting function. Also the option to download all the set of gene-associated stoichiometric reactions for a specific organism from the KEGG database <http://www.genome.jp/kegg/> is available.

Imports KEGGREST, minval (>= 0.5), sybil

License GPL-2

LazyData TRUE

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NeedsCompilation no

Author Daniel Osorio [aut, cre],
Kelly Botero [aut],
Janneth Gonzalez [aut, ths],
Andres Pinzon [aut]

Maintainer Daniel Osorio <dcosorioh@unal.edu.co>

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R topics documented:

`additionCost` *Calculate the cost of addition of a stoichiometric reaction in a metabolic network*

Description

For a given set of stoichiometric reactions this function calculates the cost of addition in a reference metabolic network. The cost is calculated by dividing the amount of non included metabolites in the reference metabolic network over the total number of metabolites involved in the reaction.

Usage

```
additionCost(reaction, reference)
```

Arguments

`reaction`	A stoichiometric reaction with the following format: `"H2O[c] + Urea-1-carboxylate[c] <=> 2 CO2[c] + 2 NH3[c]"` Where arrows and plus signs are surrounded by a "space character". It is also expected that stoichiometry coefficients are surrounded by spaces, (nothe the "2" before the CO2[c] or the NH3[c]). It also expects arrows to be in the form "=>" or "<=>". Meaning that arrows like "==>", "<==>", "-->" or "->" will not be parsed and will lead to errors.
`reference`	A set of stoichiometric reaction with the same format of reaction.

Author(s)

Daniel Camilo Osorio <dcosorioh@unal.edu.co>

Examples

```
## Not run:
# Downloading stoichiometric reactions of reference
hsa <- getReference(organism = "hsa")

# Calculating cost
additionCost(reaction = "alpha-Amino acid + H2O + NAD+ <=> 2-Oxo acid + Ammonia + NADH + H+",
             reference = hsa$reaction)

## End(Not run)
```

blockedReactions *Identify blocked reactions in a metabolic network*

Description

A blocked reaction in a metabolic network is a reaction that not participate in any optimization solution. This function set as objective function each one of the reactions (one by time) in the model, and identifies the reactions without flux under all scenarios.

Usage

```
blockedReactions(model)
```

Arguments

model	A valid model for the 'sybil' package. An object of class modelorg.

Value

A vector with the reaction ids of the blocked reactions

Author(s)

Andres Pinzon-Velasco <ampinzonv@unal.edu.co> - Mantainer: Daniel Camilo Osorio <dcosorioh@unal.edu.co>

Examples

```
## Not run:
# Loading a model for the 'sybil' package
data("Ec_core")

# Identifying blocked reactions
blockedReactions(Ec_core)
## End(Not run)
```

gapFill *Find and fill gaps in a metabolic network*

Description

This function identifies the gaps and fills it from the stoichiometric reactions of a reference metabolic reconstruction using a weighting function.

Usage

```
gapFill(reactionList, reference, limit = 0.25, woCompartment = FALSE,
  consensus = FALSE)
```

Arguments

reactionList	A set of stoichiometric reaction with the following format: "H2O[c] + Urea-1-carboxylate[c] <=> 2 CO2[c] + 2 NH3[c]" Where arrows and plus signs are surrounded by a "space character". It is also expected that stoichiometry coefficients are surrounded by spaces, (nothe the "2" before the CO2[c] or the NH3[c]). It also expects arrows to be in the form "=>" or "<=>". Meaning that arrows like "==>", "<==>", "-->" or "->" will not be parsed and will lead to errors.
reference	A set of stoichiometric reaction with the same format of reactionList
limit	An addition cost value to be used as a limit to select reactions to be added. Is calculated as NumberNewMetabolites/NumerOfMetabolites for each reaction.
woCompartment	A boolean value TRUE to define if compartment labels should be removed of the reactionList stoichiometric reactions, FALSE is used as default.
consensus	A boolean value TRUE to define if reactionList and newReactions should be reported as a unique vector or FALSE if just newReactions should be reported.

Author(s)

Kelly Botero <kjboteroo@unal.edu.co> - Maintainer: Daniel Camilo Osorio <dcosorioh@unal.edu.co>

See Also

additionCost function documentation.

Examples

```
## Not run:
# Downloading stoichiometric reactions
all <- getReference(organism = "all",sep = ";")
eco <- getReference(organism = "eco",sep = ";")

# Filtering reactions
all <- mapReactions(reactionList = all$reaction%in%eco$reaction,
                    referenceData = all,
                    by = "bool",
                    inverse = TRUE)

# gapFill
gapFill(reactionList = eco$reaction,
        reference = all$reaction,
        limit = 0.25,
        woCompartment = TRUE,
        consensus = FALSE)
## End(Not run)
```

`getReference` *Download all the set of gene-associated stoichiometric reactions for a specific organism from the KEGG database*

Description

This function downloads all the gene-associated stoichiometric reactions for a given organism from the KEGG database. If not valid organism identifier is given, all reactions from the KEGG database are downloaded. GPR are constructed using the KEGG KO association for each enzyme in a specific organism.

Usage

```
getReference(organism = "all", sep = ";")
```

Arguments

`organism`	A valid organism identifier for the KEGG database. List of valid organism identifiers are available in: http://rest.kegg.jp/list/organism . If no given, all KEGG stoichiometric reactions are downloaded.
`sep`	A character string to separate the terms.

Value

A data.frame with the following data associated to the stoichiometric reactions for a given organism:

- `ko:` The associated KEGG KO identifier to the reaction. In KEGG, molecular-level functions are stored in the KO (KEGG Orthology) database and associated with ortholog groups in order to enable extension of experimental evidence in a specific organism to other organisms.
- `id:` The associated reaction id from the KEGG database.
- `reaction:` The gene-associated stoichiometric reactions with the following format:

  `"H2O + Urea-1-carboxylate <=> 2 CO2 + 2 NH3"`

  Where arrows and plus signs are surrounded by a "space character", and stoichiometry coefficients are surrounded by spaces, (nothe the "2" before the CO2 or the NH3). Arrows will be in the form "=>" or "<=>". KEGG reactions are not compartmentalized.
- `gpr:` The Gene-Protein-Reaction (GPR) associations for a specific organism buit from the KEGG KO identifiers.

Author(s)

Kelly Johana Botero <kjboteroo@unal.edu.co> - Mantainer: Daniel Camilo Osorio <dcosorioh@unal.edu.co>

See Also

The KEGG database webpage: http://www.genome.jp/kegg/

Examples

```
## Not run:
getReference(organism = "hsa",sep = ";")

## End(Not run)
```

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