Package 'exp2flux'

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Type Package

Title Convert Gene EXPression Data to FBA FLUXes

Version 0.1

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Description For a given metabolic model with well formed Gene-Protein-Reaction (GPR) associations and an expressionSet with their associated gene expression values, this package converts gene expression values to the FBA boundaries for each reaction based in the boolean rules described in its associated GPR.

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Imports sybil, gage, igraph

Suggests Biobase

LazyData TRUE

RoxygenNote 5.0.1

NeedsCompilation no

Repository CRAN

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R topics documented:

exp2flux *Convert gene expression data to FBA fluxes*

Description

This function calculates the flux boundaries for each reaction based in their associated GPR. The value es obtained as follows: When two genes are associated by an AND operation according to the GPR rule, a min function is applied to their associated expression values. In the AND case, downregulated genes alter the reaction acting as enzyme formation limitant due two are required to complex formation. In turn, when the genes are associated by an OR rule, each one of then can code an entire enzyme to act as reaction catalyst. In this case, a sum function is applied for their associated expression values.To missing gene expression values, the function assigns one of: 'min', '1q', 'mean', 'median', '3q', or 'max' expression value calculated from the genes associated to the same metabolic pathway. In case of not possible pathway assignment to a gene, the value is calculated from all gene expression values. The fluxes boundaries of exchange reactions are not modified.

Usage

```
exp2flux(model, expression, organism = NULL, typeID = NULL,
  missing = "mean", scale = FALSE)
```

Arguments

model	A valid model for the 'sybil' package.
expression	A valid ExpressionSet object (one by treatment).
organism	A valid organism identifier for the KEGG database. List of valid organism identifiers are available in: http://rest.kegg.jp/list/organism.
typeID	A string to define the type of ID used in GPR's. One of "entrez" or "kegg" must be given.
missing	A character string specifying the value to be used in missing cases; must be one of 'min', '1q', 'mean', 'median', '3q', or 'max'
scale	A boolean value to specify if data must be scaled to assign a value of 1000 as max.

Author(s)

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Examples

```
## Not run:
# Loading a model
library("sybil")
library("Biobase")
```

```
# Original model:
data("Ec_core")

# Original model evaluation:
optimizeProb(Ec_core)

# Generating simulated expressionSets
expressionData <- matrix(data = runif(3*length(Ec_core@allGenes),min = 1,max = 100),
                         nrow = length(Ec_core@allGenes),
                         dimnames = list(c(Ec_core@allGenes),c()))
expressionData <- ExpressionSet(assayData = expressionData)

# Applying exp2flux
Ec_coreGE <- exp2flux(model = Ec_core,
                      expression = expressionData,
                      missing = "mean")
# Evaluating exp2flux model
optimizeProb(Ec_coreGE)

## End(Not run)
```

`fluxDifferences` *Report the fold change of fluxes between two models*

Description

This functions calculates the fold change `"(fluxModel2/fluxModel1)-1"` for the fluxes of two given metabolic models.

Usage

```
fluxDifferences(model1, model2, foldReport = 2)
```

Arguments

`model1`	A valid model for the `'sybil'` package.
`model2`	A valid model for the `'sybil'` package. Must have the same reactions (reaction number and reaction identifiers) as `"model1"` with different restrictions.
`foldReport`	A threshold value to be reported. All reactions with a greater or equal fold change than the given threshold are reported.

Author(s)

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Examples

```
## Not run:
# Loading a model
library("sybil")
library("Biobase")
data("Ec_core")

# Generating expressionSets
expressionData <- matrix(data = runif(3*length(Ec_core@allGenes),min = 1,max = 100),
                         nrow = length(Ec_core@allGenes),
                         dimnames = list(c(Ec_core@allGenes),c()))
expressionData <- ExpressionSet(assayData = expressionData)

# Applying exp2flux
Ec_coreGE <- exp2flux(model = Ec_core,
                      expression = expressionData,
                      missing = "mean")

# Evaluating Differences
fluxDifferences(model1 = Ec_core,
                model2 = Ec_coreGE,
                foldReport = 0.5)

## End(Not run)
```

`plotDifferences` *Plot the fold change of fluxes between two models into a bipartite graph.*

Description

This functions calculates the fold change `"(fluxModel2/fluxModel1)-1"` for the fluxes of two given metabolic models and plot it into a bipartite graph. Vertex size is assigned proportional to the fold change; if fold change is positive, green color is assigned, in contrary case, red color is assigned.

Usage

```
plotDifferences(model1, model2, ...)
```

Arguments

`model1`	A valid model for the `'sybil'` package.
`model2`	A valid model for the `'sybil'` package. Must have the same reactions (reaction number and reaction identifiers) as `"model1"` with different restrictions.
`...`	Additional arguments affecting the plot

Author(s)

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Examples

```
## Not run:
# Loading a model
library("sybil")
library("Biobase")
data("Ec_core")

# Generating expressionSets
expressionData <- matrix(data = runif(3*length(Ec_core@allGenes),min = 1,max = 100),
                         nrow = length(Ec_core@allGenes),
                         dimnames = list(c(Ec_core@allGenes),c()))
expressionData <- ExpressionSet(assayData = expressionData)

# Applying exp2flux
Ec_coreGE <- exp2flux(model = Ec_core,
                      expression = expressionData,
                      missing = "mean")

# Plotting Differences
plotDifferences(model1 = Ec_core,
                model2 = Ec_coreGE)

## End(Not run)
```

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