

Package ‘CoRegFlux’

September 29, 2020

Type Package

Title CoRegFlux

Version 1.4.0

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Description CoRegFlux aims at providing tools to integrate reverse engineered gene regulatory networks and gene-expression into metabolic models to improve prediction of phenotypes, both for metabolic engineering, through transcription factor or gene (TF) knock-out or overexpression in various conditions as well as to improve our understanding of the interactions and cell inner-working.

License GPL-3

Encoding UTF-8

LazyData false

SystemRequirements GLPK (>= 4.42)

Depends R (>= 3.6)

Imports CoRegNet, sybil

RoxygenNote 6.1.1

Suggests glpkAPI, testthat, knitr, rmarkdown, digest, R.cache,
ggplot2, plyr, igraph, methods, latex2exp,
rBayesianOptimization

biocViews GeneRegulation,Network,SystemsBiology,GeneExpression,Transcription,GenePrediction

VignetteBuilder knitr

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

git_branch RELEASE_3_11

git_last_commit 1ce49af

git_last_commit_date 2020-04-27

Date/Publication 2020-09-28

R topics documented:

adjust_constraints_to_observed_rates	2
aliases_SC	3
build_exchange_met	3

coreflux_static	4
get_biomass_flux_position	5
get_fba_fluxes_from_observations	5
get_fva_intervals_from_observations	6
get_linear_model	7
get_metabolites_exchange_fluxes	8
iMM904	8
ODCurveToFluxCurves	9
ODCurveToMetabolicGeneCurves	10
ODcurveToMetCurve	11
ODtoflux	11
ODToFluxBounds	11
PredictedGeneState	12
predict_linear_model_influence	12
SC_experiment_influence	13
SC_EXP_DATA	14
SC_GRN_1	14
SC_Test_data	15
Simulation	15
Simulation_Step	17
update_fluxes_constraints_geneKOOV	18
update_fluxes_constraints_influence	19
update_uptake_fluxes_constraints_metabolites	20
visFluxCurves	20
visMetabolicGeneCurves	21

Index 22

adjust_constraints_to_observed_rates

Adjust the constraint of the model to observed rates

Description

Adjust the constraint of the model to observed rates

Usage

```
adjust_constraints_to_observed_rates(model, metabolites_with_rates,
    exchange_met = build_exchange_met(model), backward_fluxes = "_b",
    forward_fluxes = "_f")
```

Arguments

model	a genome-scale metabolic model of class <code>modelorg</code>
metabolites_with_rates	is a <code>data.frame</code> consisting of the name of the metabolites, their concentrations and rates in <code>mmol/gDW/h</code> . The column name must be "name", "concentrations", "rates"
exchange_met	Optional. a <code>data.frame</code> as given by <code>build_exchange_met</code>
backward_fluxes	Optional. Useful for irreversible model
forward_fluxes	Optional. Useful for irreversible model

Value

Return the model with updated bounds corresponding to the observed rates provided

Examples

```
data("iMM904")
metabolites_rates<-data.frame(name=c("D-Glucose", "Glycerol"),
                             concentrations=c(16,0), rates=c(-2.81, -8.01))
iMM904_adjusted<-adjust_constraints_to_observed_rates(iMM904,
metabolites_rates)
```

aliases_SC

aliases_SC data

Description

A data.frame containing the gene ID used in the metabolic model and their common name, used in the gene regulatory network

Usage

```
aliases_SC
```

Format

a two columns data.frame which first columns correspond to the name used in the model and the second to the ID used in the GRN (common name). Those columns should be named geneName_model and geneName_GRN respectively.

geneName_model Aliases or gene names used in the gene-association field in the genome-scale metabolic model

geneName_GRN Aliases or gene names used in the gene regulatory network

build_exchange_met

Build the exchange metabolite data.frame

Description

Build the exchange metabolite data.frame

Usage

```
build_exchange_met(model)
```

Arguments

model An object of class modelOrg, the genome scale metabolic model

Value

a data.frame containing the exchange metabolite model id and the equivalent name

Examples

```
data("iMM904")
exchanged_met<-build_exchange_met(iMM904)
head(exchanged_met)
```

coreflux_static	<i>Update the model using the provided gene regulatory network and expression</i>
-----------------	---

Description

coreflux_static() uses the gene states to update the fluxes bounds from the metabolic model.

Usage

```
coreflux_static(model, predicted_gene_expression, gene_parameter = 0,
  tol = 1e-10, aliases = NULL)
```

Arguments

model	A genome-scale metabolic model of class modelorg
predicted_gene_expression	The vector of predicted gene expression for the genes present in the metabolic model as given by predict_linear_model_influence()
gene_parameter	Parameter of the softplus function
tol	Fluxes values below this threshold will be ignored.
aliases	a data.frame containing the gene names currently used in the network under the colname "geneName" and the alias under the colnames "alias"

Value

list containing:

model	the metabolic model with the coreflux constraints added
softplus_positive	the results of evaluating $\ln(1+\exp(\text{gpr}(x+\text{theta})))$ where gpr() are the continuous version of the gpr rules applied to a set of gene expression x
softplus_negative	the results of evaluating $\ln(1+\exp(\text{gpr}(x+\text{theta})))$ where gpr() are the continuous version of the gpr rules applied to a set of gene expression x

Examples

```
data("SC_GRN_1")
data("SC_experiment_influence")
data("SC_EXP_DATA")
data("aliases_SC")
data(iMM904)
data(PredictedGeneState)
static_list<-coreflux_static(iMM904,PredictedGeneState)
```

get_biomass_flux_position
Get biomass flux position

Description

Get biomass flux position

Usage

```
get_biomass_flux_position(model, biomass_reaction_id = "biomass",  
  biomass_reaction_name = NULL)
```

Arguments

model An object of class modelOrg, the genome scale metabolic model
biomass_reaction_id Default value "biomass"
biomass_reaction_name Optional, the react_name in the modelOrg under which the biomass function
 can be found, such as "growth"

Value

the position of the biomass generating reaction according the the objective in our case we had the biomass reactions for models iMM904 and iT0977

Examples

```
data("iMM904")  
get_biomass_flux_position(iMM904)
```

get_fba_fluxes_from_observations
Get fluxes balance from an observed growth rate

Description

Get fluxes balance from an observed growth rate

Usage

```
get_fba_fluxes_from_observations(model, observed_growth_rate,  
  metabolites_rates = NULL,  
  biomass_flux_index = get_biomass_flux_position(model),  
  backward_fluxes = "_b", forward_fluxes = "_f")
```

Arguments

model a genome-scale metabolic model of class `modelorg`
observed_growth_rate a numerical value for the observed growth rate
metabolites_rates Optional, a `data.frame` consisting of the name of the metabolites, their concentrations and rates in mmol/gDW/h to adjust the model uptake rates. The column name must be "name", "concentrations", "rates"
biomass_flux_index Optional. Index of the biomass flux as returned by `get_biomass_flux_position()`
backward_fluxes Optional, only relevant for irreversible model
forward_fluxes Optional, only relevant for irreversible model

Value

Return fluxes values compatible with the observed growth rate through flux balance analysis

Examples

```

data("iMM904")
metabolites_rates<-data.frame(name=c("D-Glucose","Glycerol"),
                             concentrations=c(16,0),rates=c(-2.81,-8.01))

FluxesFromObs<-get_fba_fluxes_from_observations(iMM904,0.205,
metabolites_rates = metabolites_rates)
  
```

get_fva_intervals_from_observations

Get intervals of flux variability (FVA) from an observed growth rate

Description

Get intervals of flux variability (FVA) from an observed growth rate

Usage

```

get_fva_intervals_from_observations(model, observed_growth_rate,
  metabolites_rates = NULL,
  biomass_flux_index = get_biomass_flux_position(model))
  
```

Arguments

model a genome-scale metabolic model of class `modelorg`
observed_growth_rate a numerical value for the observed growth rate
metabolites_rates Optional. a `data.frame` consisting of the name of the metabolites, their concentrations and rates in mmol/gDW/h to adjust the model uptake rates. The column name must be "name", "concentrations", "rates"
biomass_flux_index Optional. Index of the biomass flux as returned by `get_biomass_flux_position()`

Value

Return the interval of fluxes values compatible with the observed growth rate through flux variability analysis

Examples

```
data("iMM904")
metabolites_rates<-data.frame(name=c("D-Glucose", "Glycerol"),
                             concentrations=c(16,0),rates=c(-2.81,-8.01))

FluxesVarFromObs<-get_fva_intervals_from_observations(iMM904,0.205,
metabolites_rates=metabolites_rates)
```

<code>get_linear_model</code>	<i>Train a linear model</i>
-------------------------------	-----------------------------

Description

Here we train a linear regression model of the form $x = \alpha + \beta * I$ where x is the gene expression of the metabolic genes of the train data set `train_expression`, α is an intercept, I is the influence of the regulators of the training data set and β are the coefficients.

Usage

```
get_linear_model(train_expression,
  train_influence = regulatorInfluence(network, train_expression, minTarg
  = 10), network)
```

Arguments

<code>train_expression</code>	Gene expression of the training data set, not necessary if <code>train_influence</code> is supplied. Should be numerical matrix corresponding to the gene expression. Rownames should contain gene names/ids while samples should be in columns.
<code>train_influence</code>	Optional. Regulator influence scores computed using the function <code>CoRegNet::regulatorInfluence</code> for the training data set, default <code>minTarg = 10</code>
<code>network</code>	<code>CoRegNet</code> object use to build the linear model and to compute the influence.

Details

`train_expression` Gene expression of the training data set, not necessary if `train_influence` is supplied. Should be numerical matrix corresponding to the gene expression. Rownames should contain gene names/ids while samples should be in columns.

Value

A linear model

See Also

`predict_linear_model_influence`

```
get_metabolites_exchange_fluxes
```

Get metabolites exchange fluxes

Description

Get metabolites exchange fluxes

Usage

```
get_metabolites_exchange_fluxes(model, metabolites,
  exchange_met = build_exchange_met(model), backward_fluxes = "_b",
  forward_fluxes = "_f")
```

Arguments

model	An object of class modelOrg, the genome scale metabolic model
metabolites	A data.frame containing the names and concentrations of metabolites
exchange_met	A data.frame as build by the function build_exchange_met
backward_fluxes	Optional parameter for irreversible model to indicate backward fluxes
forward_fluxes	Optional parameter for irreversible model to indicate forward fluxes

Value

a data.frame containing the exchange metabolite model id and the equivalent name

Examples

```
data("iMM904")
metabolites<-data.frame("name"=c("D-Glucose","Glycerol"),
  "concentrations"=c(16,0))
get_metabolites_exchange_fluxes(iMM904,metabolites)
```

```
iMM904
```

```
iMM904
```

Description

A *S. cerevisiae*_ genome-scale metabolic model as a modelOrg object

Usage

```
iMM904
```

Format

a modelOrg object as required by `_sybil_`. See `_sybilSBML_` for more information on how to load other model.

 ODCurveToFluxCurves *ODCurveToFluxCurves*

Description

This function takes measured ODs and turn them into a FluxCurves object to be visualize using `visFluxCurves()`. It relies on flux variability analysis to highlight the flux value interval required to meet the specified OD.

Usage

```
ODCurveToFluxCurves(model, ODs, times, metabolites_rates = NULL,
  biomass_flux_index = get_biomass_flux_position(model))
```

Arguments

<code>model</code>	An object of class <code>modelOrg</code> , the metabolic model.
<code>ODs</code>	A vector of measured ODs
<code>times</code>	A vector of timepoints at which the flux balance analysis solution will be evaluated.
<code>metabolites_rates</code>	A data.frame containing the extraneous metabolites, their initial concentrations and their uptake rates. Columns must be named "names", "concentrations" and "rates".
<code>biomass_flux_index</code>	Optional. index of the flux corresponding to the biomass reaction.

Value

An object `FluxCurves` to visualize using the function `visFluxCurves`

See Also

`visFluxCurves`, `ODCurveToMetabolicGeneCurves`, `visMetabolicGeneCurves`

Examples

```
data(iMM904)
ODs<-seq.int(0.099,1.8,length.out = 5)
times = seq(0.5,2,by=0.5)

metabolites_rates <- data.frame("name"=c("D-Glucose"),
  "concentrations"=c(16.6), "rates"=c(-2.81))

ODtoflux<-ODCurveToFluxCurves(model = iMM904,
  ODs = ODs,times = times, metabolites_rates = metabolites_rates)

visFluxCurves(ODtoflux)
```

 ODCurveToMetabolicGeneCurves

ODCurveToMetabolicGeneCurves

Description

This function takes measured ODs and turn them into a ODCurveToMetCurve object to be visualize using `visMetabolicGeneCurves()`. It relies on flux variability analysis to highlight the flux value interval required to meet the specified OD and to map it on the metabolic genes.

Usage

```
ODCurveToMetabolicGeneCurves(times, ODs, metabolites_rates = NULL, model,
  softplusParam = 0, singlePointFluxEstimate = FALSE,
  biomass_flux_index = get_biomass_flux_position(model),
  aliases = NULL)
```

Arguments

<code>times</code>	A vector of timepoints at which the flux balance analysis solution will be evaluated.
<code>ODs</code>	vector of measured ODs.
<code>metabolites_rates</code>	A data.frame containing the extraneous metabolites, their initial concentrations and their uptake rates. Columns must be named "names", "concentrations" and "rates".
<code>model</code>	An object of class <code>modelOrg</code> , the metabolic model.
<code>softplusParam</code>	Softplus parameter identify through calibration.
<code>singlePointFluxEstimate</code>	Optional, logical.
<code>biomass_flux_index</code>	index of the flux corresponding to the biomass reaction.
<code>aliases</code>	Optional. A data.frame containing the gene names used in the metabolic model and the aliases to use to match the regulatory network.

Value

Metabolic genes curves to visualize using the function `visMetabolicGeneCurves`

Examples

```
ODs<-c(0.4500000,0.5322392,0.6295079,0.7445529)
data("aliases_SC","iMM904")
ODcurveToMetCurve<-ODCurveToMetabolicGeneCurves(times = seq(0.5,2,by=0.5),
  ODs = ODs,model = iMM904,aliases = aliases_SC)
visMetabolicGeneCurves(ODcurveToMetCurve,genes="YJR077C")
```

ODcurveToMetCurve	<i>ODcurveToMetCurve data</i>
-------------------	-------------------------------

Description

List as obtained by the function `ODCurveToMetabolicGeneCurves`

Usage

`ODcurveToMetCurve`

Format

List as obtained by the function `ODCurveToMetabolicGeneCurves`

ODtoflux	<i>ODtoflux data</i>
----------	----------------------

Description

List as obtained by the function `ODCurveToFluxCurves`

Usage

`ODtoflux`

Format

List as obtained by the function `ODCurveToFluxCurves`

ODToFluxBounds	<i>ODToFluxBounds</i>
----------------	-----------------------

Description

`ODToFluxBounds`

Usage

```
ODToFluxBounds(odRate, model, metabolites_rates = NULL,
               biomass_flux_index = get_biomass_flux_position(model))
```

Arguments

odRate	The values of OD measured over time
model	An object of class modelOrg, the metabolic model.
metabolites_rates	A data.frame containing the extraneous metabolites, their initial concentrations and their uptake rates. Columns must be named "names", "concentrations" and "rates".
biomass_flux_index	Optional. index of the flux corresponding to the biomass reaction.

Value

Flux bounds from OD

PredictedGeneState	<i>PredictedGeneState data</i>
--------------------	--------------------------------

Description

Predicted gene states as obtained by the function `predict_linear_model_influence`

Usage

PredictedGeneState

Format

a named vector containing the gene name and its associated predicted gene state.

<code>predict_linear_model_influence</code>	<i>Predict the gene expression level based on condition-specific influence</i>
---	--

Description

Build a linear model and use it to predict the gene expression level from the influence of an experiment

Usage

```
predict_linear_model_influence(network, model,
  train_influence = regulatorInfluence(network, train_expression,
  min_Target), experiment_influence, train_expression, min_Target = 10,
  tol = 1e-10, aliases = NULL, verbose = 0)
```

Arguments

network	a coregnet object
model	A genome-scale metabolic model from a class modelOrg.
train_influence	Optional, if is train_expression is provided. An influence matrix as computed by the function regulatorInfluence() from CoRegNet
experiment_influence	Regulator influence scores for the condition of interest as a named vector with the TF as names.
train_expression	Gene expression of the training data set, not necessary if train_influence is supplied. Should be numerical matrix corresponding to the gene expression. Row-names should contain gene names/ids while samples should be in columns.
min_Target	Optional. Use in case train_influence is not provided. Default value = 10. See regulatorInfluence for more information.
tol	Fluxes values below this threshold will be ignored. Default
aliases	Optional, A two columns data.frame containing the name used in the gene regulatory network and their equivalent in the genome-scale metabolic model to allow the mapping of the GRN onto the GEM. The colnames should be geneName_model and geneName_GRN
verbose	Default to 0. Give informations about the process status

Value

The predicted genes expressions/states

Examples

```

data("SC_GRN_1")
data("SC_experiment_influence")
data("SC_EXP_DATA")
data("iMM904")
data("aliases_SC")
PredictedGeneState <- predict_linear_model_influence(network = SC_GRN_1,
  experiment_influence = SC_experiment_influence,
  train_expression = SC_EXP_DATA,
  min_Target = 4,
  model = iMM904,
  aliases= aliases_SC)

GeneState<-data.frame("Name"=names(PredictedGeneState),
  "State"=unname(PredictedGeneState))

```

SC_experiment_influence

SC_experiment_influence data

Description

A vector of influence computed from the first sample of SC_Test_data

Usage

SC_experiment_influence

Format

a named numerical vector

SC_EXP_DATA	<i>SC_EXP_DATA data</i>
-------------	-------------------------

Description

A matrix of *S. cerevisiae* gene expression in various experimental designs, derived from the m3d dataset to infer *S. cerevisiae* gene regulatory network. The dataset was shortened to 3600 genes in order to limit the size of the object

Usage

SC_EXP_DATA

Format

a matrix of 3600 genes by 247 samples

Source

subset of m3d dataset available at <<http://m3d.mssm.edu/>>

SC_GRN_1	<i>SC_GRN_1 data</i>
----------	----------------------

Description

A coregnet object inferred from the m3d dataset describing the gene regulatory network for *S. cerevisiae* as described in Banos, D. T., Trébulle, P., & Elati, M. (2017). Integrating transcriptional activity in genome-scale models of metabolism. *BMC systems biology*, 11(7), 134.

Usage

SC_GRN_1

Format

a coregnet object inferred using the package `_CoRegNet_`

Number of transcription factor 200

Number of targets genes 3748

Evidences TRUE ...

SC_Test_data	<i>SC_Test_data data</i>
--------------	--------------------------

Description

A matrix of *S. cerevisiae* gene expression during diauxic shift (Brauer and al.)

Usage

```
SC_Test_data
```

Format

a matrix of 6028 genes by 13 samples during diauxic shift

Source

E-GEOD-4398 (Brauer MJ and al.)

Simulation	<i>Simulation using Dynamic Flux balance analysis over time as in varma</i>
------------	---

Description

Simulation using Dynamic Flux balance analysis over time as in *varma*

Usage

```
Simulation(model, time = c(0, 1), metabolites, initial_biomass,
  biomass_flux_index = CoRegFlux::get_biomass_flux_position(model),
  coregnet = NULL, regulator_table = NULL, gene_table = NULL,
  gene_state_function = NULL, time_step_fba_bounds = NULL,
  softplus_parameter = 0, aliases = NULL)
```

Arguments

model	An object of class <code>modelOrg</code> , the genome-scale metabolic model (GEM).
time	Timepoints at which the flux balance analysis solution will be evaluated.
metabolites	A <code>data.frame</code> containing the extraneous metabolites and the initial concentrations
initial_biomass	The value of the biomass at the beginning of the simulation
biomass_flux_index	index of the flux corresponding to the biomass reaction.
coregnet	Object of class <code>CoRegNet</code> , containing the regulatory and coregulatory interactions.

<code>regulator_table</code>	A data.frame containing 3 columns: "regulator", "influence", "expression" containing respectively the name of a TF present in the CoRegNet object as a string, its influence in the condition of interest as a numerical and an expression factor of 0 for a KO, or an integer >1 for an overexpression
<code>gene_table</code>	A data.frame containing 2 columns: "gene" and "expression" containing respectively the name of a gene present in the modelOrg as a string and an expression factor of 0 for a KO, or an integer >1 for an overexpression
<code>gene_state_function</code>	Function to obtain the gene state for a given subset of gene
<code>time_step_fba_bounds</code>	Bounds for the fba problem at each time point, overrides any other form of constraining for a given flux.
<code>softplus_parameter</code>	the softplus parameter identify through calibration
<code>aliases</code>	Optional. A data.frame containing the gene names currently used in the network under the colname "geneName" and the alias under the colnames "alias"

Details

The simulation function allows the user to run several kind of simulations based on the provided arguments. When providing only the GEM, time, initial biomass and the metabolites, a classical dFBA is carried out. To integrate the gene expression to the GEM, the `gene_state_function` must be provided while if the user wants to simulate a TF knock-out or overexpression, then a `coregnet` object and the `regulator` table should also be provided. See the vignette and quick-user guide for more examples.

Value

Return a list containing the simulation information such as the `objective_history`, `fluxes_history`, `met_concentration_history`, `biomass_history`

Examples

```
data("SC_GRN_1")
data("SC_EXP_DATA")
data("SC_experiment_influence")
data("iMM904")
data("aliases_SC")
data("PredictedGeneState")

metabolites<-data.frame("name"=c("D-Glucose", "Glycerol"),
                       "concentrations"=c(16,0))

result_without_any_constraint<-Simulation(iMM904, time=seq(1,10,by=1),
                                         metabolites,
                                         initial_biomass=0.45,
                                         aliases = aliases_SC)

GeneState<-data.frame("Name"=names(PredictedGeneState),
                     "State"=unname(PredictedGeneState))

result<-Simulation(iMM904, time=seq(1,10,by=1),
                  metabolites,
```



```

        initial_biomass=0.45,
        gene_state_function=function(a,b){GeneState},
        aliases = aliases_SC)

result$biomass_history

```

Simulation_Step *Single simulation step*

Description

Single simulation step in which fluxes are reconstrained according to metabolite concentrations, then given the continuous evaluation of the gpr rules and the softplus function of the gene regulatory state.

Usage

```

Simulation_Step(model, coregnet, metabolites, met_concentrations_t0,
  biomass_t0, regulator_table, gene_table, time_step, gene_state,
  softplus_parameter, aliases, biomass_flux_index)

```

Arguments

model	An object of class modelOrg, the metabolic model.
coregnet	Optional, object of class CoRegNet object containing the information about regulatory and coregulatory relationships
metabolites	data frame of metabolites names
met_concentrations_t0	data frame of metabolites concentrations at t0, before performing a time step
biomass_t0	biomass at t0 before performing a step
regulator_table	A data.frame containing 3 columns: "regulator", "influence", "expression" containing respectively the name of a TF present in the CoRegNet object as string, its influence in the condition of interest as a numerical and an expression factor of 0 for a KO, or an integer >1 for an overexpression
gene_table	A data.frame containing 2 columns: "gene", "expression" containing respectively the name of a gene present in the CoRegNet object as string and an expression factor of 0 for a KO, or an integer >1 for an overexpression
time_step	size of the time step to perform; that is t1-t0
gene_state	data frame with rows being gene names and columns being the gene expression or any other continuous value representing metabolites activity to be evaluated using the gpr rules
softplus_parameter	Softplus parameter identify through calibration. Default to 0.
aliases	Optional. A data.frame containing the gene names currently used in the network under the colname "geneName" and the alias under the colnames "alias"
biomass_flux_index	index of the flux corresponding to the biomass reaction.

Value

list of: fluxes: fluxes of the resulting fba solution to the metabolic and genetic constraints biomass_yield: biomass yield that is used as proxy for the growth rate in the dynamic flux balance analysis solution. Corresponds to the flux of the biomass reaction of the model.

See Also

Simulation

update_fluxes_constraints_geneKOOV

Update the fluxes constraints to simulate gene KO or overexpression

Description

Update the constraints of the reactions associated with the knock-out or overexpressed gene

Usage

```
update_fluxes_constraints_geneKOOV(model, gene_table, aliases = NULL)
```

Arguments

model	An object of class modelOrg, the metabolic model.
gene_table	A data.frame containing 2 columns: "gene", "expression" containing respectively the name of a gene present in the CoRegNet object as string and an expression factor of 0 for a KO, or an integer >1 for an overexpression
aliases	Optional. A data.frame containing the gene names used in the metabolic model and the aliases to use to match the regulatory network

Value

Return the model with updated bounds

Examples

```
data("iMM904")
data("aliases_SC")
gene_table <- data.frame("gene" = c("YGL202W", "YIL162W"),
  "expression" =c(2,0), stringsAsFactors = FALSE)

model_gene_KO_OV_constraints <- update_fluxes_constraints_geneKOOV(
  model= iMM904,
  gene_table = gene_table,
  aliases = aliases_SC)
```

 update_fluxes_constraints_influence

Update the fluxes constraints to simulate TF KO or overexpression

Description

Update the constraints according to the influence & regulatory network for a single KO or overexpression

Usage

```
update_fluxes_constraints_influence(model, coregnet, regulator_table,
  aliases)
```

Arguments

model	An object of class modelOrg, the metabolic model.
coregnet	Object of class CoRegNet, containing the regulatory and coregulatory interactions.
regulator_table	A data.frame containing 3 columns: "regulator", "influence", "expression" containing respectively the name of a TF present in the CoRegNet object as string, its influence in the condition of interest as a numerical and an expression factor of 0 for a KO, or an integer >1 for an overexpression
aliases	Optional, a data.frame containing the gene names used in the metabolic model and the aliases to use to match the regulatory network

Value

Return the model with updated bounds

Examples

```
data("SC_GRN_1")
data("iMM904")
data("aliases_SC")
regulator_table <- data.frame("regulator" = "MET32",
  "influence" = -1.20322 ,
  "expression" = 3,
  stringsAsFactors = FALSE)
model_TF_KO_OV_constraints <- update_fluxes_constraints_influence(
  model= iMM904, coregnet = SC_GRN_1, regulator_table = regulator_table,
  aliases = aliases_SC)
```

update_uptake_fluxes_constraints_metabolites

Update the fluxes constraints given the metabolite concentrations

Description

Update the fluxes constraints given the metabolite concentrations

Usage

```
update_uptake_fluxes_constraints_metabolites(model, met_fluxes_indexes,
      met_concentrations_t0, biomass_t0, time_step)
```

Arguments

model	An object of class modelOrg, the metabolic model.
met_fluxes_indexes	Indexes of the metabolites fluxes
met_concentrations_t0	Metabolites concentrations at t0
biomass_t0	Biomasss at t0
time_step	time_step studied

Value

Return the updated model

visFluxCurves

Visualize Fluxes Curves

Description

Visualize Fluxes Curves

Usage

```
visFluxCurves(fluxCurves, genes = unique(fluxCurves$name)[seq_len(50)],
  ...)
```

Arguments

fluxCurves	result table from ODCurveToFluxCurves
genes	a vector containing the names of the metabolic genes to plot. Default select the first 50 genes
...	Optional others curves

Value

a plot of the curves of the chosen fluxes

See Also

ODCurveToFluxCurves, ODCurveToMetabolicGeneCurves, visMetabolicGeneCurves

Examples

```
data("ODtoflux")
visFluxCurves(ODtoflux, genes = "ADK3")
```

visMetabolicGeneCurves

Visualize Metabolic Gene Curves

Description

Visualize Metabolic Gene Curves

Usage

```
visMetabolicGeneCurves(metabCurves,
  genes = unique(metabCurves$name)[seq_len(50)], ...)
```

Arguments

metabCurves	result table from ODCurveToMetabolicGeneCurves
genes	a vector containing the names of the metabolic genes to plot. Default select the first 50 genes
...	Optional, others curves

Value

a plot of the curves of the chosen metabolic genes

See Also

ODCurveToMetabolicGeneCurves, ODCurveToFluxCurves, visFluxCurves

Examples

```
data("ODcurveToMetCurve")
visMetabolicGeneCurves(ODcurveToMetCurve, genes="YJR077C")
```

Index

* datasets

- aliases_SC, [3](#)
 - iMM904, [8](#)
 - ODcurveToMetCurve, [11](#)
 - ODtoflux, [11](#)
 - PredictedGeneState, [12](#)
 - SC_EXP_DATA, [14](#)
 - SC_experiment_influence, [13](#)
 - SC_GRN_1, [14](#)
 - SC_Test_data, [15](#)
- adjust_constraints_to_observed_rates, [2](#)
- aliases_SC, [3](#)
- build_exchange_met, [3](#)
- coregflux_static, [4](#)
- get_biomass_flux_position, [5](#)
- get_fba_fluxes_from_observations, [5](#)
- get_fva_intervals_from_observations, [6](#)
- get_linear_model, [7](#)
- get_metabolites_exchange_fluxes, [8](#)
- iMM904, [8](#)
- ODCurveToFluxCurves, [9](#)
- ODCurveToMetabolicGeneCurves, [10](#)
- ODcurveToMetCurve, [11](#)
- ODtoflux, [11](#)
- ODToFluxBounds, [11](#)
- predict_linear_model_influence, [12](#)
- PredictedGeneState, [12](#)
- SC_EXP_DATA, [14](#)
- SC_experiment_influence, [13](#)
- SC_GRN_1, [14](#)
- SC_Test_data, [15](#)
- Simulation, [15](#)
- Simulation_Step, [17](#)
- update_fluxes_constraints_geneKOOV, [18](#)
- update_fluxes_constraints_influence, [19](#)
- update_uptake_fluxes_constraints_metabolites, [20](#)
- visFluxCurves, [20](#)
- visMetabolicGeneCurves, [21](#)