

# Package ‘CoRegFlux’

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**Type** Package

**Title** CoRegFlux

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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)

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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 modelorg
metabolites_with_rates	is a data.frame consisting of the name of the metabolites, their concentrations and rates in mmol/gDW/h. The column name must be "name", "concentrations", "rates"
exchange_met	Optional. a data.frame as given by build_exchange_met
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 `iTO977`

**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`,  $\alpha$  is an intercept,  $I$  is the influence of the regulators of the training data set and  $\beta$  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>
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---

**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 shorten 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.

regulator_table	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
gene_table	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
gene_state_function	Function to obtain the gene state for a given subset of gene
time_step_fba_bounds	Bounds for the fba problem at each time point, overrides any other form of constraining for a given flux.
softplus_parameter	the softplus parameter identify through calibration
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"

### 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")
```

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