

Cahier des charges

Communication et conception d'un projet de recherche et/ou
développement

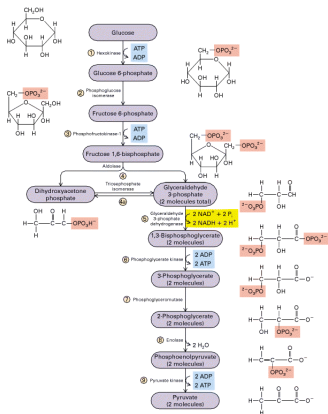
Arnaud FRÈCHE
Charlotte HÉRICÉ
Saraï MOLA
Typhaine PAYSAN-LAFOSSE
Joris SANSEN

Master 2 BioInformatique

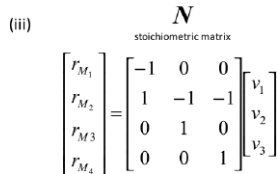
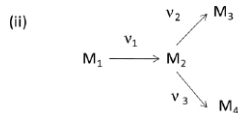
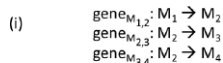
5 Décembre 2012

Introduction

Réseaux Métaboliques



Modes Élémentaires



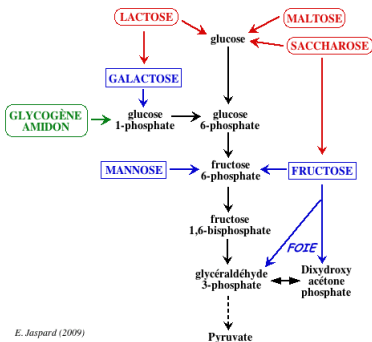
Contexte

Sujet

- Calcul de flux
- *regEfmtool*

Objectifs

- Interface Graphique
- Technologies Web



E. Jaspard (2009)

État de l'existant

CellNetAnalyser

- Package de MATLAB
- Analyse fonctionnelle et structurale de réseaux biochimiques
- Calcul des modes élémentaires grâce à METATOOL

Edit reaction

Reaction identifier (use "mue" for biomass synthesis):
 PYR::AcCoA

Reaction equation (examples: A + 2 B = C ; = A):
 1 Pyr = 1 AcCoA + 1 NADH + 1 CO2

Default rate (# for empty): #

Rate minimum (0=Irrevers.): 0

Rate maximum: 100

Coeff. in objective function: 0

Variance of measurements: 0.01

Notes and Comments:

Flux map number: Map 1: Cataboli...
 Text box style: Editable

X-Position: 266
 Y-Position: 761
 Get x/y-Pos

OK Cancel

État de l'existant

METATOOL

- Étude structure réseaux métaboliques
- Calcul des modes élémentaires
- Module de MATLAB
- Format entrée : fichier *.dat*, format sortie : fichier *.out*

RegEfmsTool

- Extension d'*EfmsTool*
- Calcul des modes élémentaires de flux
- Régulation transcriptionnelle du réseau métabolique
- Fichiers textes formatés en entrée

Besoins fonctionnels

Besoins fonctionnels

- Interface Homme-Machine
- Chargement des données
- Réglage des paramètres et aide utilisateur
- Résultats

Maquette



Maquette

WebEfmtool

Create network

Load network

Modify network

Help

Create network

network name :

list of metabolites :

metabolite 1	ok	X
metabolite 2	ok	X
<input type="text"/>	ok	X
<input type="text"/>	ok	X
<input type="text"/>	ok	X
<input type="text"/>	ok	X
<input type="text"/>	ok	X
<input type="text"/>	ok	X

list of enzymes :

enzyme 1	ok	X
enzyme 2	ok	X
<input type="text"/>	ok	X
<input type="text"/>	ok	X

list of co-factors :

co-factor 1	ok	X
co-factor 2	ok	X
<input type="text"/>	ok	X
<input type="text"/>	ok	X

Return

Validate

Maquette

WebEfmtool

Create network

Load network

Modify network

Help

Create Reactions

reaction name :

reagents of the reaction	stoichiometry
<input type="text" value="reagent"/> ▼	<input type="text" value="1.25"/>
<input type="text" value="reagent"/> ▼	<input type="text" value="1.25"/>
<input type="text" value="reagent"/> ▼	<input type="text" value="1.25"/>
<input type="button" value="add more"/>	

enzymes
<input type="text" value="enzyme"/> ▼
<input type="button" value="add more"/>
Co-factors
<input type="text" value="co-factor 1"/> ▼
<input type="text" value="1.25"/>
<input type="button" value="add more"/>

products of the reaction	stoichiometry
<input type="text" value="product 1"/> ▼	<input type="text" value="1.25"/>
<input type="text" value="product 2"/> ▼	<input type="text" value="1.25"/>
<input type="text" value="product 3"/> ▼	<input type="text" value="1.25"/>
<input type="button" value="add more"/>	

reversibility : ☐ yes ☐ no

Maquette

WebEfmttool

Create network

Load network

Modify network

Help

Load a network

metabolites file :

met file

browse

reactions file :

reactions file

browse

reversibility file :

reversibility file

browse

stoichiometry file :

stoichiometry file

browse

reactions reversibility file :

reactions reversibility file

browse

generule file :

generule file

browse

return

validate

Maquette

WebEfmtreeol

Create network

Load network

Modify network

Help

Run WebEfmtreeol

Simulation options

Results display

☐ on WebEfmtreeol

☐ save in a text file

Kind of stoichiometric file :

☐ flux-analyser-dir

☐ flux-analyser-files

☐ reaction-list

☐ excel

☐ stoichiometry

☐ sbml

Output options :

☐ null

☐ count

☐ text-boolean

☐ text-doubles

☐ binary-boolean

☐ binary-doubles

☐ matlab

Results view options :

☒ metabolites

☒ reactions

☒ unique flux

☒ iterations

☒ stoich matrix

☒ kernel matrix

Run

Maquette

WebEfmtreeol

Create network

Load network

Modify network

Help

Run WebEfmtreeol

Results

Network metabolites :

M_13dpg_c, M_2pg_c, M_3pg_c, M_6pgc_c, M_6pgl_c, M_ac_c, M_ac_b, M_acald_c, M_accoa_c, M_acon_c, M_actp_c, M_adp_c, M_akg_c, M_amp_c, M_ara_L_c, M_ara_L_b, M_atp_c, M_atpmain_b, M_cit_c, M_co2_c, M_co2_b, M_coa_c, M_dd6pg_c, M_dhap_c, M_e4p_c, M_etoh_c, M_etoh_b, M_f6p_c, M_fdp_c, M_for_c, M_for_b, M_fru_b, M_fum_c, M_fum_b, M_g3p_c, M_g6p_c, M_gal_c, M_gal_b, M_glc_D_b, M_glx_c, M_h2_b, M_icit_c, M_lac_D_c, M_lac_D_b, M_m6p_c, M_mal_L_c, M_mal_L_b, M_man_b, M_nad_c, M_nadh_c, M_nadp_c, M_nadph_c, M_nh4_c, M_nh4_b, M_o2_b, M_o2_c, M_oaa_c, M_peg_c, M_pyr_c, M_pyr_b, M_q8_c, M_q8h2_c, M_r5p_c, M_ru5p_D_c, M_s7p_c, M_succ_c, M_succ_b, M_succoa_c, M_xu5p_D_c, M_xylo_c, M_xylo_b, M_xyly_c,

Network reactions :

R_PG1: M_g6p_c <=> M_f6p_c
R_PFK: M_atp_c + M_f6p_c -> M_adp_c + M_fdp_c
R_FBP: M_fdp_c -> M_f6p_c
R_FBA: M_fdp_c <=> M_dhap_c + M_g3p_c
R_TPI: M_dhap_c <=> M_g3p_c
R_GAPD: M_g3p_c + M_nad_c <=> M_13dpg_c + M_nadh_c
R_PGK: M_3pg_c + M_atp_c <=> M_13dpg_c + M_adp_c
R_PGM: M_2pg_c <=> M_3pg_c
R_ENO: M_2pg_c <=> M_peg_c
R_PYK: M_adp_c + M_peg_c -> M_atp_c + M_pyr_c
R_PPS: M_atp_c + M_pyr_c -> M_amp_c + M_peg_c

Compare

Maquette

WebEfmtreeol

Create network

Load network

Modify network

Help

Run WebEfmtreeol

Results

Network metabolites :

M_13dpg_c, M_2pg_c, M_3pg_c, M_6pgc_c, M_6pgl_c, M_ac_c, M...
 M_acon_c, M_actp_c, M_adp_c, M_akg_c, M_amp_c, M_ara_L...
 M_cit_c, M_co2_c, M_co2_b, M_coa_c, M_dd6pg_c, M_dhap_c, M...
 M_f6p_c, M_fdp_c, M_for_c, M_for_b, M_fru_b, M_fum_c, M_fum_b...
 M_gal_b, M_glc_D_b, M_glx_c, M_h2_b, M_icit_c, M_lac_D_c, M_la...
 M_mal_L_b, M_man_b, M_nad_c, M_nadh_c, M_nadp_c, M_nadph...
 M_o2_c, M_oaa_c, M_pep_c, M_pyr_c, M_pyr_b, M_q8_c, M_q8h2...
 M_s7p_c, M_succ_c, M_succ_b, M_succoa_c, M_xu5p_D_c, M_xyl...

Network reactions :

R_PG1: M_g6p_c <=> M_f6p_c
 R_PFK: M_atp_c + M_f6p_c -> M_adp_c + M_fdp_c
 R_FBP: M_fdp_c -> M_f6p_c
 R_FBA: M_fdp_c <=> M_dhap_c + M_g3p_c
 R_TPI: M_dhap_c <=> M_g3p_c
 R_GAPD: M_g3p_c + M_nad_c <=> M_13dpg_c + M_nadh_c
 R_PGK: M_3pg_c + M_atp_c <=> M_13dpg_c + M_adp_c
 R_PGM: M_2pg_c <=> M_3pg_c
 R_ENO: M_2pg_c <=> M_pep_c
 R_PYK: M_adp_c + M_pep_c -> M_atp_c + M_pyr_c
 R_PPS: M_atp_c + M_pyr_c -> M_amp_c + M_pep_c

Network metabolites :

M_13dpg_c, M_2pg_c, M_3pg_c, M_6pgc_c, M_6pgl_c, M_ac_c, M...
 M_acon_c, M_actp_c, M_adp_c, M_akg_c, M_amp_c, M_ara_L...
 M_cit_c, M_co2_c, M_co2_b, M_coa_c, M_dd6pg_c, M_dhap_c, M...
 M_f6p_c, M_fdp_c, M_for_c, M_for_b, M_fru_b, M_fum_c, M_fum_b...
 M_gal_b, M_glc_D_b, M_glx_c, M_h2_b, M_icit_c, M_lac_D_c, M_la...
 M_mal_L_b, M_man_b, M_nad_c, M_nadh_c, M_nadp_c, M_nadph...
 M_o2_c, M_oaa_c, M_pep_c, M_pyr_c, M_pyr_b, M_q8_c, M_q8h2...
 M_s7p_c, M_succ_c, M_succ_b, M_succoa_c, M_xu5p_D_c, M_xyl...

Network reactions :

R_PG1: M_g6p_c <=> M_f6p_c
 R_PFK: M_atp_c + M_f6p_c -> M_adp_c + M_fdp_c
 R_FBP: M_fdp_c -> M_f6p_c
 R_FBA: M_fdp_c <=> M_dhap_c + M_g3p_c
 R_TPI: M_dhap_c <=> M_g3p_c
 R_GAPD: M_g3p_c + M_nad_c <=> M_13dpg_c + M_nadh_c
 R_PGK: M_3pg_c + M_atp_c <=> M_13dpg_c + M_adp_c
 R_PGM: M_2pg_c <=> M_3pg_c
 R_ENO: M_2pg_c <=> M_pep_c
 R_PYK: M_adp_c + M_pep_c -> M_atp_c + M_pyr_c
 R_PPS: M_atp_c + M_pyr_c -> M_amp_c + M_pep_c

Compare

Besoins non fonctionnels

Besoins non fonctionnels

- Portabilité
- Sécurité et robustesse
- Temps de calcul
- Documentation

Choix et justifications

Langages

- Structure (squelette du site) = HTML
- Design = CSS
- Interactivité = JavaScript
- Communication avec Base de données = PHP

Choix et justifications

Accessibilité

- Différents niveaux d'utilisation possibles : basique ou avancé
- Séparation de la partie graphique et de la partie calculs
- Documentation