

Cahier des charges

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

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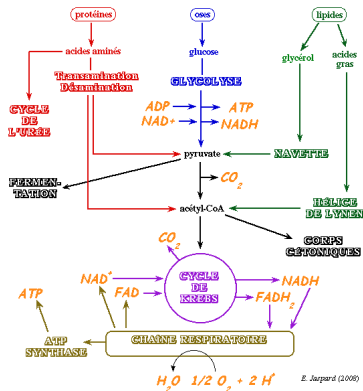
Master 2 BioInformatique

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Introduction

- Réseaux Métaboliques
- Modes Élémentaires



Contexte

Sujet

- Calcul de flux
- *regEfmtool*

Objectifs

- Interface Graphique
- Technologies Web

État de l'existant

RegEfmtool

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

CellNetAnalyser

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

État de l'existant

MetaTool

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="button" value="v"/> | <input type="text" value="1.25"/> |
| <input type="text" value="reagent"/> <input type="button" value="v"/> | <input type="text" value="1.25"/> |
| <input type="text" value="reagent"/> <input type="button" value="v"/> | <input type="text" value="1.25"/> |
| <input type="button" value="add more"/> | |

| enzymes |
|---|
| <input type="text" value="enzyme"/> <input type="button" value="v"/> |
| <input type="button" value="add more"/> |
| Co-factors |
| <input type="text" value="co-factor 1"/> <input type="button" value="v"/> |
| <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="button" value="v"/> | <input type="text" value="1.25"/> |
| <input type="text" value="product 2"/> <input type="button" value="v"/> | <input type="text" value="1.25"/> |
| <input type="text" value="product 3"/> <input type="button" value="v"/> | <input type="text" value="1.25"/> |
| <input type="button" value="add more"/> | |

reversibility : ☐ yes ☐ no

Maquette

WebEfmtool

Create network

Load network

Modify network

Help

Load a network

metabolites file :

reactions file :

reversibility file :

stoichiometry file :

reactions reversibility file :

generule file :

Maquette

WebEfmtool

Create network

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Modify network

Help

Run WebEfmtool

Simulation options

Results display

☐ on WebEfmtool

☐ 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_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_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
- Animation, interactivité = Javascript
- Communication avec Base de données = PHP

Choix et justifications

Accessibilité