Cahier des charges

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

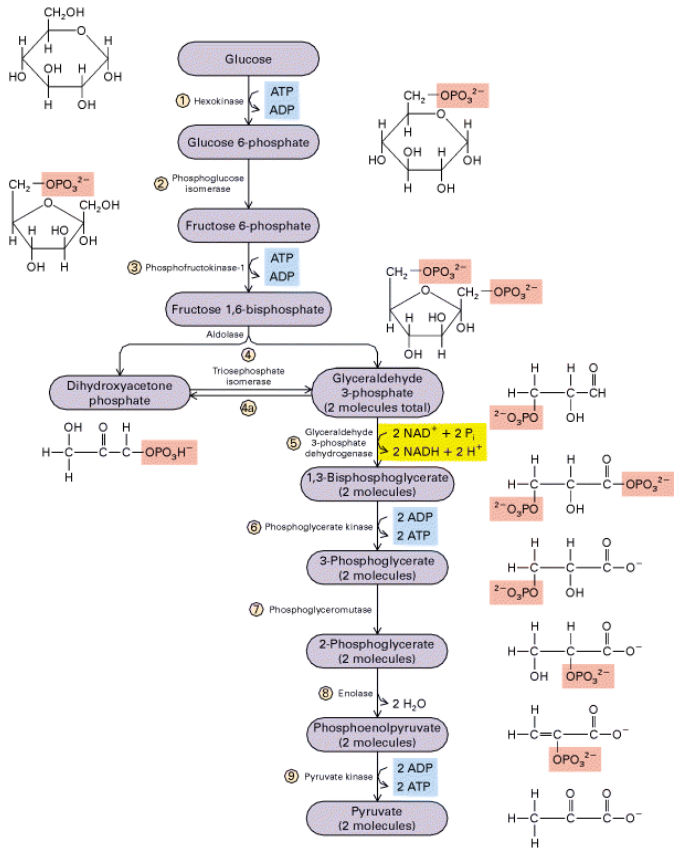
Arnaud Frèche
Charlotte Hériché
Sarai Mola
Typhaine Paysan-Lafosse
Joris Sansen

Master 2 BioInformatique

5 Décembre 2012

Introduction

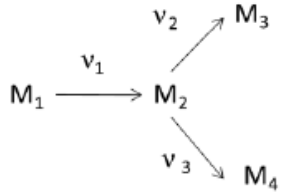
- Réseaux Métaboliques
- Modes Élémentaires



(i)

$$gene_{M_{1,2}}: M_1 \rightarrow M_2$$
$$gene_{M_{2,3}}: M_2 \rightarrow M_3$$
$$gene_{M_{3,4}}: M_2 \rightarrow M_4$$

(ii)



(iii)

$$\boldsymbol{N}$$

stoichiometric matrix

$$\begin{bmatrix} r_{M_1} \\ r_{M_2} \\ r_{M3} \\ r_{M_4} \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

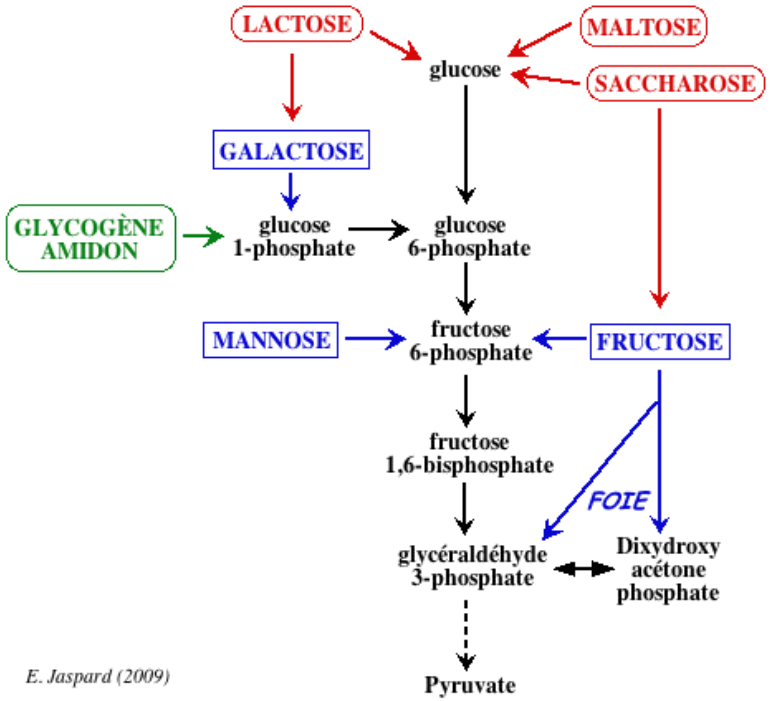
Contexte

Sujet

- Calcul de flux
- *regEfmtool*

Objectifs

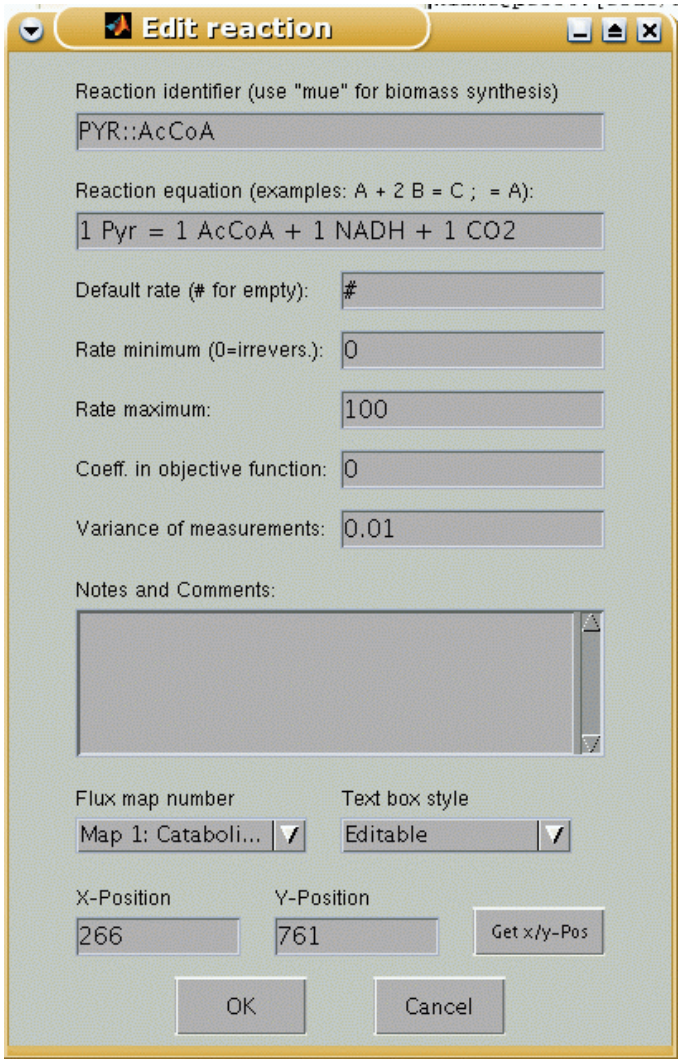
- Interface Graphique
- Technologies Web



État de l'existant

CellNetAnalyser

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



État de l'existant

MetaTool

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

RegEfmtool

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

Besoins fonctionnels

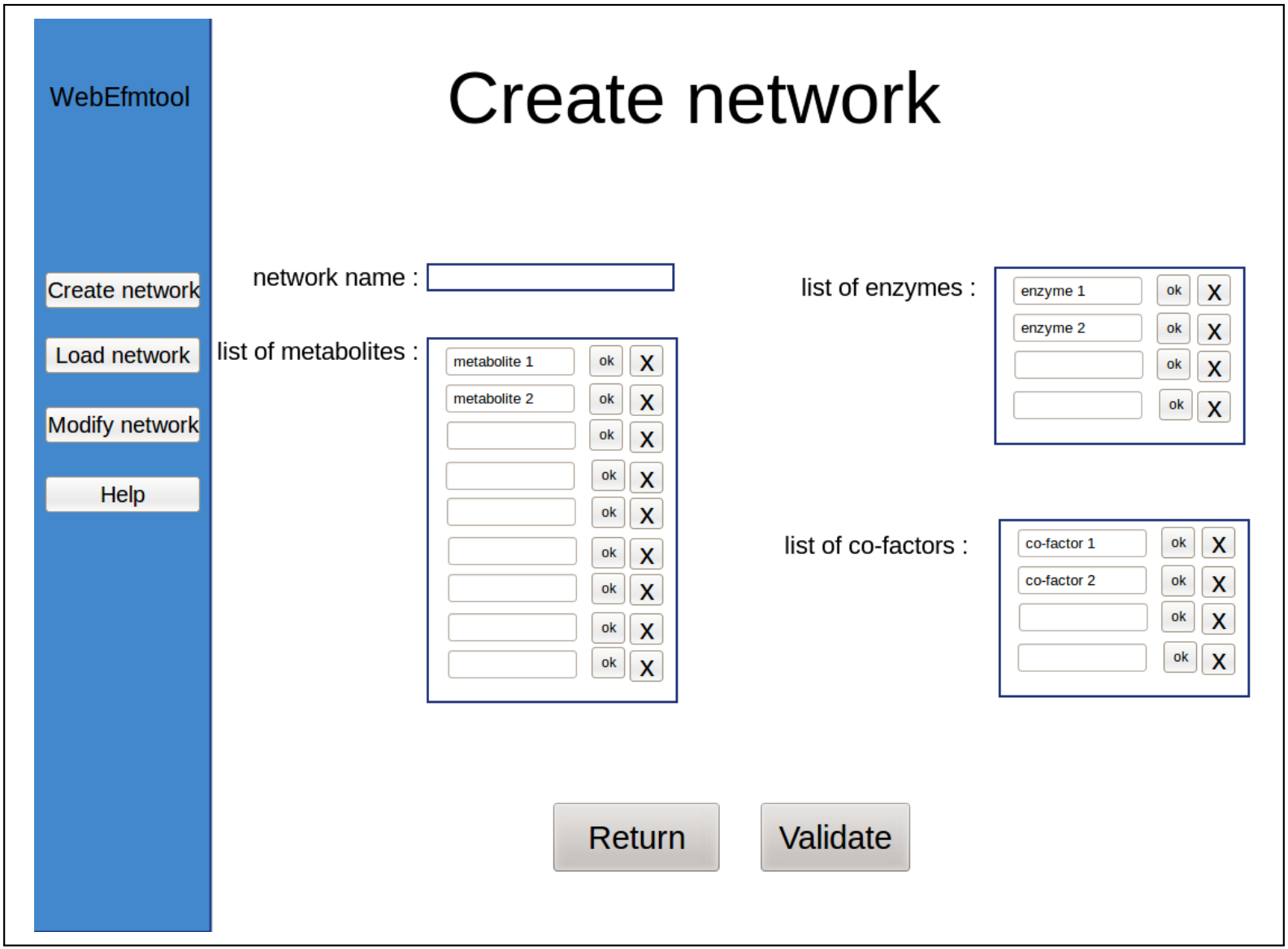
Besoins fonctionnels

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

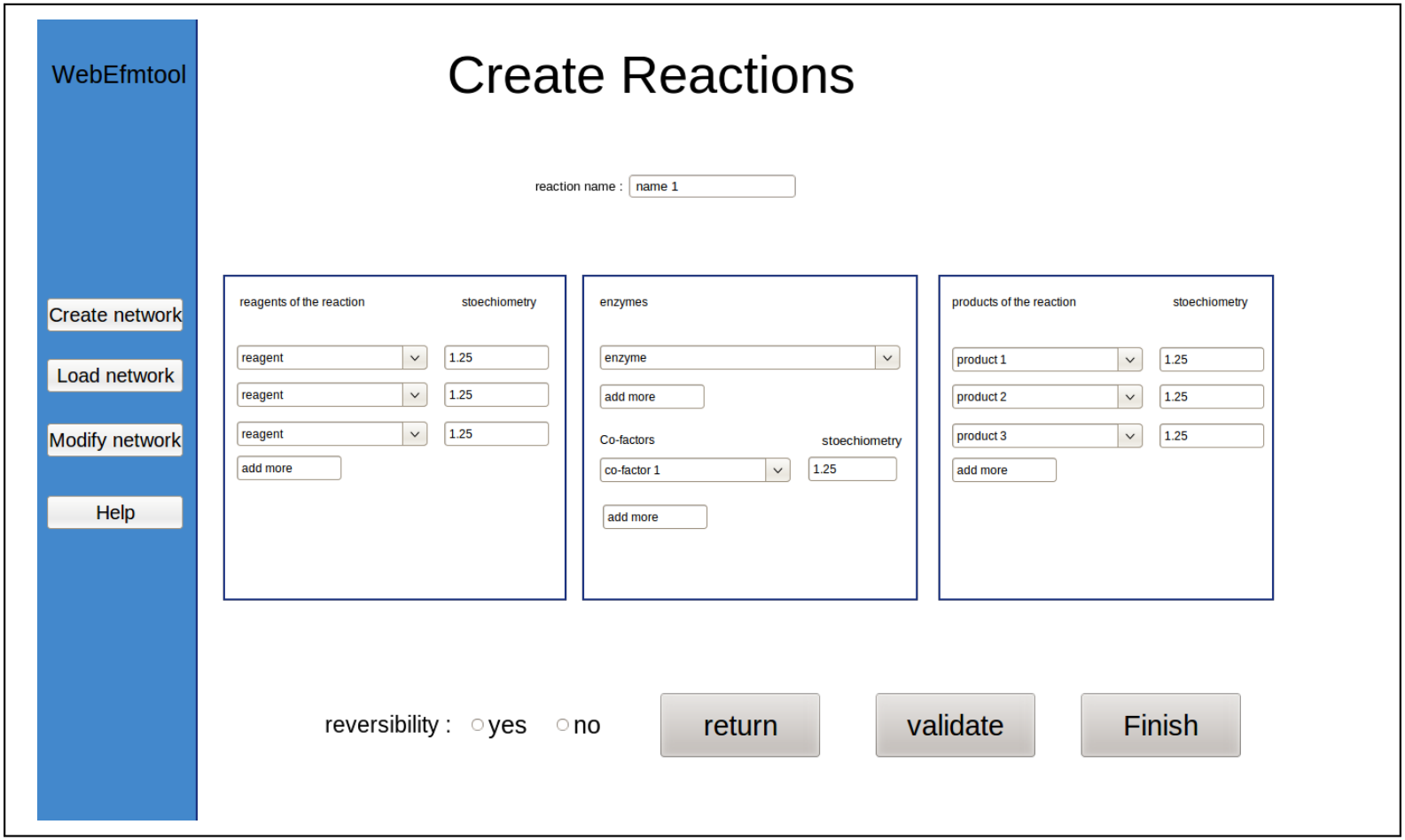
Maquette


WebEfmtool
Welcome on WebEfmtool !
This new tool will help you to use RegEfmtool
modeling software, create manage and modify network,
make simulation on your web browser
and on any OS system !
New network
Load network
Modify network
Help

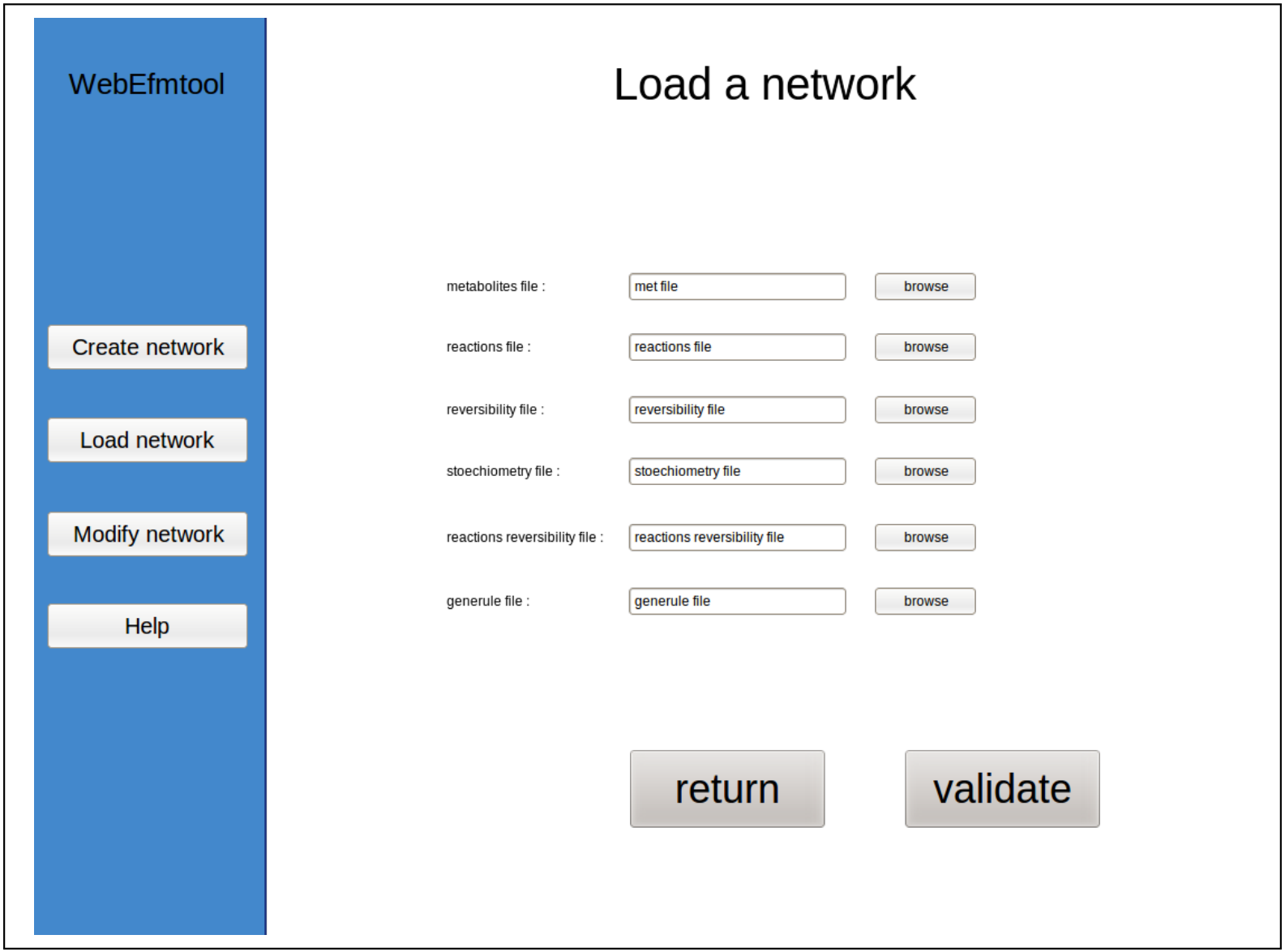
Maquette


WebEfmtool
Create network
Load network
Modify network
Help
Create network
network name :
list of metabolites :
metabolite 1
metabolite 2
ok
X
list of enzymes :
enzyme 1
enzyme 2
list of co-factors :
co-factor 1
co-factor 2
Return
Validate

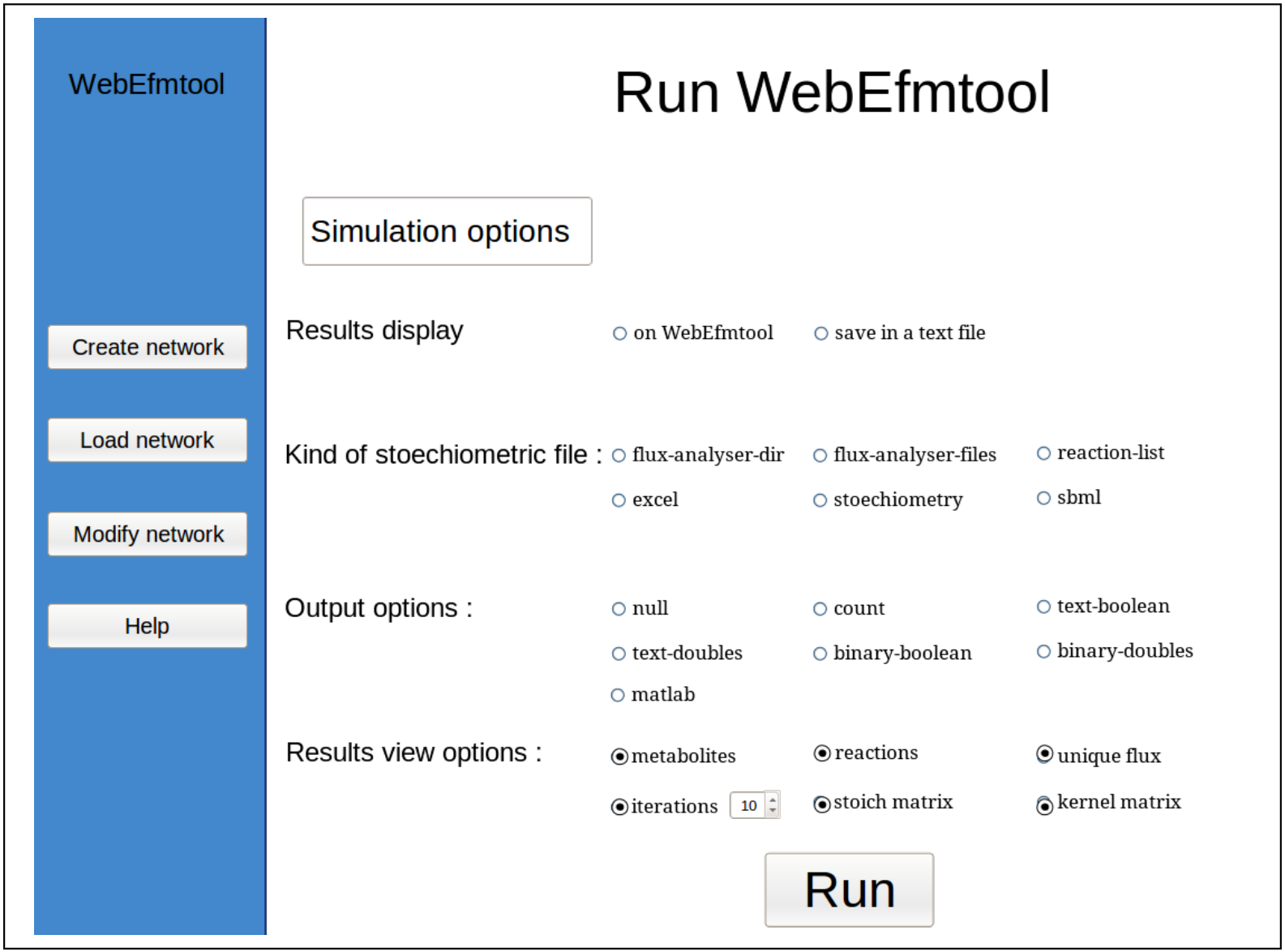
Maquette


WebEfmtool
Create network
Load network
Modify network
Help
Create Reactions
reaction name : name 1
reagents of the reaction
stoechiometry
reagent
1.25
reagent
1.25
reagent
1.25
add more
enzymes
enzyme
add more
Co-factors
stoechiometry
co-factor 1
1.25
add more
products of the reaction
stoechiometry
product 1
1.25
product 2
1.25
product 3
1.25
add more
reversibility :
yes
no
return
validate
Finish

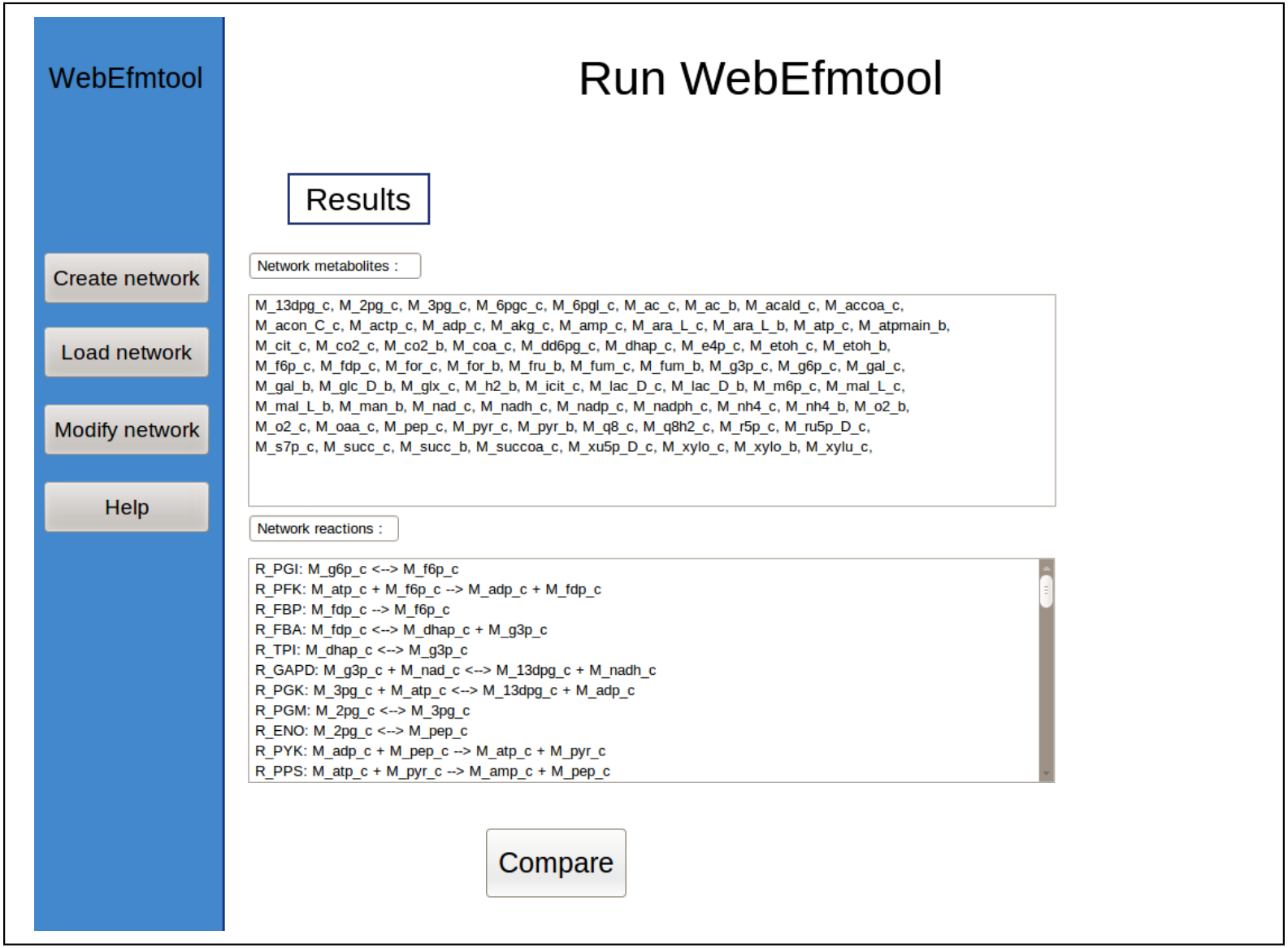
Maquette


WebEfmtool
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
stoechiometry file :
stoechiometry file
browse
reactions reversibility file :
reactions reversibility file
browse
generule file :
generule file
browse
return
validate

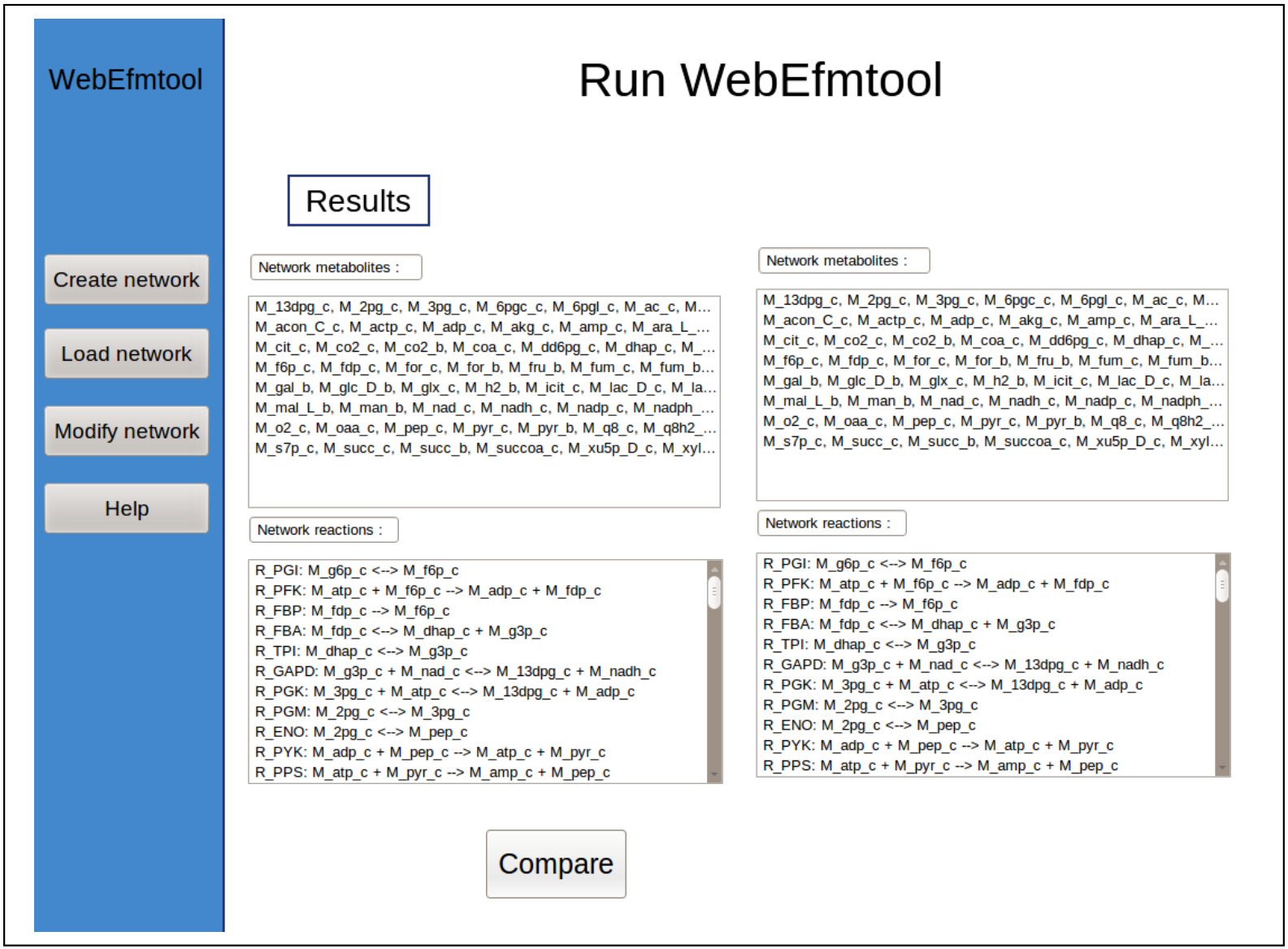
Maquette


WebEfmtool
Create network
Load network
Modify network
Help
Run WebEfmtool
Simulation options
Results display
on WebEfmtool
save in a text file
Kind of stoechiometric file :
flux-analyser-dir
flux-analyser-files
reaction-list
excel
stoechiometry
sbml
Output options :
null
count
text-boolean
text-doubles
binary-boolean
binary-doubles
matlab
Results view options :
metabolites
reactions
unique flux
iterations
10
stoich matrix
kernel matrix
Run

Maquette


WebEfmtool
Create network
Load network
Modify network
Help
Run WebEfmtool
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_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_pep_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_xylu_c,
Network reactions :
R_PGI: 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

Maquette


WebEfmtool
Create network
Load network
Modify network
Help
Run WebEfmtool
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...
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R_ENO: M_2pg_c <--> M_pep_c
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R_PPS: M_atp_c + M_pyr_c --> M_amp_c + M_pep_c
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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 :
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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