

Electronic Supplementary Information for: Dynamic elementary mode modelling of non-steady state flux data

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1 Metabolic models.

1.1 Simulated case study

Metabolite abbreviations

Abbreviation	Metabolite
GLCo	Glucose
GLCi	Glucose (intracellular)
Prb	Energy status
G6P	Glucose-6-phosphate
F6P	Fructose 1,6-phosphate
Glyc	Glycogen
PHOS	Phosphate

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Trh	Trehalose
F16P	Fructose-6-biphosphate
TRIO	Triose-phosphates
NAD	Nicotinamide adenine dinucleotide
BPG	Bisphosphoglycerate
NADH	Nicotinamide adenine dinucleotide phosphate
P3G	3-Phosphoglycerate
P2G	2-Phosphoglycerate
PEP	Phosphoenolpyruvate
PYR	Pyruvate
ACE	Acetate
CO2	Carbon dioxide
SUCC	Succinate
ETOH	Ethanol
X	Polyphosphates

List of reactions

$GLCi + Prb \leftrightarrow G6P$
 $G6P \leftrightarrow F6P$
 $G6P + Prb \leftrightarrow Glyc + 2 PHOS$
 $Prb + 2 G6P \leftrightarrow Trh + 3 PHOS$
 $F6P + Prb \leftrightarrow F16P$
 $F16P \leftrightarrow 2 TRIO$
 $PHOS + TRIO + NAD \leftrightarrow BPG + NADH$
 $BPG \leftrightarrow P3G + Prb$
 $P3G \leftrightarrow P2G$
 $P2G \leftrightarrow PEP$
 $PEP \leftrightarrow Prb + PYR; F16P$
 $PYR \leftrightarrow ACE + CO2$
 $2 ACE + 3 NAD \leftrightarrow SUCC + 3 NADH$
 $GLCo \leftrightarrow GLCi$
 $ACE + NADH \leftrightarrow ETOH + NAD$
 $NADH + TRIO \leftrightarrow PHOS + GLY + NAD$
 $Prb \leftrightarrow PHOS$
 $X \leftrightarrow PHOS$

1.2 Real case study

Metabolite abbreviations

Abbreviation	Metabolite
g6p	Glucose-6-phosphate
f6p	Fructose-6-phosphate
fbp	Fructose 1,6-biphosphate
g3p	Glyceraldehydes-3-phosphate
3pg	3-Phosphoglycerate
pep	Phosphoenolpyruvate
pyr	Pyruvate
cit	Citric acid
ogl	Oxoagglutarate
succ	Succinate
fum	Fumarate
mal	Malate

List of reactions

g6p \rightarrow
g6p \leftrightarrow
g6p \leftrightarrow f6p
f6p \rightarrow fbp
fbp \rightarrow g3p
g3p \rightarrow
fbp \leftrightarrow 3pg
3pg \rightarrow
3pg \leftrightarrow pep
pep \rightarrow
pep \rightarrow pyr
pyr \rightarrow
pyr \rightarrow cit
cit \rightarrow ogl
ogl \leftrightarrow
ogl \rightarrow succ
succ \rightarrow
succ \rightarrow fum

fun \rightarrow mal
mal \rightarrow cit