Additional file 2 for the paper entitled:
Symbolic flux analysis for genome-scale metabolic networks

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1 Introduction

This document is a supplementary material to the above article and acts as a companion to the SBML file provided as additional file 1: yeast_example.xml. The content of this document is generated from the SBML file and acts as a convenient view of the model of yeast central metabolism. The composition of the model is discussed in the main text.

2 Contents of the SBML model of the example yeast network

2.1 Definition of all species

Legend: m - mitochondria, c - cytosol, x - external.

Symbol	Compartments	Description
AA	c, m	C00084 Acetaldehyde
AC	c, m	C00033 Acetate
AH	c	C01077 O-Acetyl-L-homoserine
ALA	c, m, x	C00041 L-Alanine
AN	c	C00108 Anthranilate
ARG	c, x	C00062 L-Arginine
AS	c	C03406 N-(L-Arginino)succinate
ASN	c, x	C00152 L-Asparagine
ASP	c, m, x	C00049 L-Aspartate
AcCoA	c, m, x	C00024 Acetyl-CoA
C	c	C00327 L-Citrulline
CH	c	C00251 Chorismate
CI	m	C00158 Citrate/Isocitrate
CO2	c, m, x	C00011 Carbon dioxide
CP	c	C00169 Carbamoyl phosphate
EivP	c	C00279 D-Erythrose 4-phosphate
FU	c, m	C00122 Fumarate
FviP	c, x	C05345 β-D-Fructose 6-phosphate
GL	c, x	C00031 D-Glucose
GLN	c, m, x	C00064 L-Glutamine
GLU	c, m, x	C00025 L-Glutamate
GLY	c, x	C00037 Glycine
GP	c	C00111 Glycerone phosphate
GiiiP	c, x	C00118 D-Glyceraldehyde 3-phosphate
GviP	c, x	C00668 α-D-Glucose 6-phosphate
HC	c	C00155 L-Homocysteine
HCO3-	c, m	C00288 Bicarbonate
HIS	c, x	C00135 L-Histidine
I	c	C00463 Indole
ILE	c, m, x	C00407 L-Isoleucine
IOS	c, m	C04236 (2S)-2-Isopropyl-3-oxosuccinate
IP	c	C03506 Indoleglycerol phosphate
LEU	c, m, x	C00123 L-Leucine
LYS	c, x	C00047 L-Lysine
MA	m	C00149 Malate
MET	c, x	C00073 L-Methionine
MO	c, m	C00141 3-Methyl-2-oxobutanoic acid

table continues ...

Table 1: (continued)

Symbol	Compartments	Description
OA	c, m, x	C00036 Oxaloacetate
OAG	c	C05533 Oxaloglutarate
OG	c, m	C00026 2-Oxoglutarate
OR	c, m	C00077 L-Ornithine
PEP	c	C00074 Phosphoenolpyruvate
PHE	c, x	C00079 L-Phenylalanine
PRO	c, x	C00148 L-Proline
PY	c, m	C00022 Pyruvate
PvRA	c	C04302 N-(5-Phospho-β-D-ribosyl)anthranilate
RLvP	c	C00199 D-Ribulose 5-phosphate
RvP	c, x	C00117 D-Ribose 5-phosphate
SER	c, x	C00065 L-Serine
SU	m	C00042 Succinate
SUCoA	m	C00091 Succinyl-CoA
SiiiP	c	C03175 Shikimate 3-phosphate
SviiP	c	C05382 D-Sedoheptulose 7-phosphate
THR	c, m, x	C00188 L-Threonine
TRP	c, x	C00078 L-Tryptophan
TYR	c, x	C00082 L-Tyrosine
VAL	c, m, x	C00183 L-Valine
XvP	c	C00231 D-Xylulose 5-phosphate
XviCPA	c	Six carbon analogue used in the CPA reaction.
YiGOG	c, m	One carbon analogue used in GLU-OG stoichiometry.
YiiXvP	c	Intermediate product of reaction R01830 (TKL1 or TKL2)
ZiiPY	m	Part of PY used in ILE, VAL, and LEU biosynthesis.
ZiiXvP	c	Intermediate product of reaction R01641 (TKL1 or TKL2)
ZiiiFviP	c	Intermediate product of reaction R01827 (TAL1)
ZivALT	c, m	Used to link the stoichiometry of the ALT reaction.
ZvAAT	c, m	Used to link the stoichiometry of the AAT1 and AAT2 reactions.
ZviGOG	c, m	Six carbon analogue used in GLU-OG stoichiometry.

2.2 Definition of all reactions

Gene	Reaction/flux	
Cytosolic reactions:		
AAo	$\xrightleftharpoons{\nu_{\text{AAo\_ACo}}}$	ACo
ACo	$\xrightleftharpoons{\nu_{\text{ACo\_AcCoAo}}}$	AcCoAo
BCo + GLNo	$\xrightleftharpoons{\nu_{\text{BCo\_CPo\_01}}}$	XviCPAo
XviCPAo	$\xrightleftharpoons{\nu_{\text{BCo\_CPo\_02}}}$	CPo + GLUo
AHo	$\xrightleftharpoons{\nu_{\text{B\_AC\_01}}}$	ACo + HCo
ASPo	$\xrightleftharpoons{\nu_{\text{B\_ASP\_ASN}}}$	ASNo
ASPo	$\xrightleftharpoons{\nu_{\text{B\_ASP\_THR}}}$	THRo
ASPo + AcCoAo	$\xrightleftharpoons{\nu_{\text{B\_AcCoA\_01}}}$	AHo
GLUo	$\xrightleftharpoons{\nu_{\text{B\_GLU\_GLN}}}$	GLNo
GLUo	$\xrightleftharpoons{\nu_{\text{B\_GLU\_PRO}}}$	PROo
SERo	$\xrightarrow{\nu_{\text{B\_GiiiP\_GLY}}}$	CO_2 + GLYo
GiiiPo	$\xrightleftharpoons{\nu_{\text{B\_GiiiP\_SER}}}$	SERo
AcCoAo + OGo	$\xrightleftharpoons{\nu_{\text{B\_LYS\_C1}}}$	OAGo
OAGo	$\xrightarrow{\nu_{\text{B\_LYS\_C2}}}$	CO_2 + LYSo
BCo + HCo	$\xrightleftharpoons{\nu_{\text{B\_OA\_AcCoA\_MET}}}$	METo
BCo + OAo	$\xrightleftharpoons{\nu_{\text{B\_OAo\_ASP\_01}}}$	ZvAATo
ZvAATo	$\xrightleftharpoons{\nu_{\text{B\_OAo\_ASP\_02}}}$	ASPo + YiGOGo
OGo	$\xrightleftharpoons{\nu_{\text{B\_OG\_GLU\_C}}}$	GLUo
PEPo + SiiiPo	$\xrightleftharpoons{\nu_{\text{B\_PEP\_01}}}$	CHo
EivPo + PEPo	$\xrightleftharpoons{\nu_{\text{B\_PEP\_EivP\_01}}}$	SiiiPo
CHo	$\xrightarrow{\nu_{\text{B\_PEP\_EivP\_PHE}}}$	CO_2 + PHEo
CHo	$\xrightleftharpoons{\nu_{\text{B\_PEP\_EivP\_TRP\_01}}}$	ANo + PYo
ANo + RvPo	$\xrightleftharpoons{\nu_{\text{B\_PEP\_EivP\_TRP\_02}}}$	PvRAo
PvRAo	$\xrightarrow{\nu_{\text{B\_PEP\_EivP\_TRP\_03}}}$	CO_2 + IPo
IPo	$\xrightleftharpoons{\nu_{\text{B\_PEP\_EivP\_TRP\_04}}}$	GiiiPo + Io
Io + SERo	$\xrightleftharpoons{\nu_{\text{B\_PEP\_EivP\_TRP\_05}}}$	TRPo
CHo	$\xrightarrow{\nu_{\text{B\_PEP\_EivP\_TYR}}}$	CO_2 + TYRo
BCo + PYo	$\xrightleftharpoons{\nu_{\text{B\_PY\_ALA\_C1}}}$	ZivALTo
ZivALTo	$\xrightleftharpoons{\nu_{\text{B\_PY\_ALA\_C2}}}$	ALAo + YiGOGo
AcCoAo + MOo	$\xrightleftharpoons{\nu_{\text{B\_PY\_AcCoA\_C}}}$	IOSo
IOSo	$\xrightarrow{\nu_{\text{B\_PY\_AcCoA\_LEU\_C}}}$	CO_2 + LEUo
MOo	$\xrightleftharpoons{\nu_{\text{B\_PY\_VAL\_C}}}$	VALo
BCo + RvPo	$\xrightleftharpoons{\nu_{\text{B\_RvP\_HIS}}}$	HISo

table continues ...

Table 2: (continued)

Gene	Reaction/flux	
THRo	$\xrightleftharpoons{\nu_{\text{B\_THR\_GLY}}}$	ACo + GLYo
CO_2	$\xrightleftharpoons{\nu_{\text{CD\_BC}}}$	BCo
FviPo	$\xrightleftharpoons{\nu_{\text{FviP\_GP\_GiiiP}}}$	GPo + GiiiPo
GLUo + YiGOGo	$\xrightleftharpoons{\nu_{\text{GLUo\_OGo\_01}}}$	ZviGOGo
ZviGOGo	$\xrightleftharpoons{\nu_{\text{GLUo\_OGo\_02}}}$	BCo + OGo
GLo	$\xrightleftharpoons{\nu_{\text{GL\_GviP}}}$	GviPo
GPo	$\xrightleftharpoons{\nu_{\text{GP\_GiiiP}}}$	GiiiPo
GiiiPo	$\xrightleftharpoons{\nu_{\text{GiiiP\_PEP}}}$	PEPo
GviPo	$\xrightleftharpoons{\nu_{\text{GviP\_FviP}}}$	FviPo
GviPo	$\xrightarrow{\nu_{\text{GviP\_RLvP}}}$	CO_2 + RLvPo
OAo	$\xrightarrow{\nu_{\text{OA\_PEP}}}$	CO_2 + PEPo
PEPo	$\xrightleftharpoons{\nu_{\text{PEP\_PY}}}$	PYo
GiiiPo + ZiiiFviPo	$\xrightleftharpoons{\nu_{\text{PPP\_FviP\_EivP\_SviiP\_GiiiP\_01}}}$	FviPo
SviiPo	$\xrightleftharpoons{\nu_{\text{PPP\_FviP\_EivP\_SviiP\_GiiiP\_02}}}$	EivPo + ZiiiFviPo
FviPo	$\xrightleftharpoons{\nu_{\text{PPP\_FviP\_GiiiP\_XvP\_EivP\_01}}}$	EivPo + YiiXvPo
GiiiPo + YiiXvPo	$\xrightleftharpoons{\nu_{\text{PPP\_FviP\_GiiiP\_XvP\_EivP\_02}}}$	XvPo
RvPo + ZiiXvPo	$\xrightleftharpoons{\nu_{\text{PPP\_SviiP\_GiiiP\_XvP\_RvP\_01}}}$	SviiPo
XvPo	$\xrightleftharpoons{\nu_{\text{PPP\_SviiP\_GiiiP\_XvP\_RvP\_02}}}$	GiiiPo + ZiiXvPo
PYo	$\xrightarrow{\nu_{\text{PYo\_AAo}}}$	AAo + CO_2
BCo + PYo	$\xrightleftharpoons{\nu_{\text{PYo\_OAo}}}$	OAo
RLvPo	$\xrightleftharpoons{\nu_{\text{RLvP\_RvP}}}$	RvPo
ARGo	$\xrightarrow{\nu_{\text{US\_ARG\_OR}}}$	CO_2 + ORo
ASo	$\xrightleftharpoons{\nu_{\text{US\_AS\_FU\_ARG}}}$	ARGo + FUo
ASPo + Co	$\xrightleftharpoons{\nu_{\text{US\_C\_ASP\_AS}}}$	ASo
CPo + ORo	$\xrightleftharpoons{\nu_{\text{US\_OR\_C}}}$	Co
XvPo	$\xrightleftharpoons{\nu_{\text{XvP\_RLvP}}}$	RLvPo
Transport reactions:		
ALAo	$\xrightarrow{\nu_{\text{ALA}_{\text{out}}}}$	ALAx
ARGo	$\xrightarrow{\nu_{\text{ARG}_{\text{out}}}}$	ARGx
ASNo	$\xrightarrow{\nu_{\text{ASN}_{\text{out}}}}$	ASNx
ASPo	$\xrightarrow{\nu_{\text{ASP}_{\text{out}}}}$	ASPx
AcCoAo	$\xrightarrow{\nu_{\text{AcCoA}_{\text{out}}}}$	AcCoAx
CO_2	$\xrightarrow{\nu_{\text{CO}_2,\text{out}}}$	CO_2

table continues ...

Table 2: (continued)

Gene	Reaction/flux	
	FviPo $\xrightarrow{\nu_{\mathrm{FviP_{out}}}}$	FviPx
	GLNo $\xrightarrow{\nu_{\mathrm{GLN_{out}}}}$	GLNx
	GLUo $\xrightarrow{\nu_{\mathrm{GLU_{out}}}}$	GLUx
	GLYo $\xrightarrow{\nu_{\mathrm{GLY_{out}}}}$	GLYx
	GLx $\xrightarrow{\nu_{\mathrm{GL_{in}}}}$	GLo
	GiiiPo $\xrightarrow{\nu_{\mathrm{GiiiP_{out}}}}$	GiiiPx
	GviPo $\xrightarrow{\nu_{\mathrm{GviP_{out}}}}$	GviPx
	HISo $\xrightarrow{\nu_{\mathrm{HIS_{out}}}}$	HISx
	ILEo $\xrightarrow{\nu_{\mathrm{ILE_{out}}}}$	ILEx
	LEUo $\xrightarrow{\nu_{\mathrm{LEU_{out}}}}$	LEUx
	LYSo $\xrightarrow{\nu_{\mathrm{LYS_{out}}}}$	LYSx
	METo $\xrightarrow{\nu_{\mathrm{MET_{out}}}}$	METx
	OAo $\xrightarrow{\nu_{\mathrm{OA_{out}}}}$	OAx
	PHEo $\xrightarrow{\nu_{\mathrm{PHE_{out}}}}$	PHEx
	PROo $\xrightarrow{\nu_{\mathrm{PRO_{out}}}}$	PROx
	RvPo $\xrightarrow{\nu_{\mathrm{RvP_{out}}}}$	RvPx
	SERo $\xrightarrow{\nu_{\mathrm{SER_{out}}}}$	SERx
	THRo $\xrightarrow{\nu_{\mathrm{THR_{out}}}}$	THRx
	TRPo $\xrightarrow{\nu_{\mathrm{TRP_{out}}}}$	TRPx
	TYRo $\xrightarrow{\nu_{\mathrm{TYR_{out}}}}$	TYRx
	VALo $\xrightarrow{\nu_{\mathrm{VAL_{out}}}}$	VALx
Cytosolic-mitochondrial transport reactions:		
	AAo $\xrightleftharpoons{\nu_{\mathrm{AAo\_AAm}}}$	AAm
	ALAm $\xrightleftharpoons{\nu_{\mathrm{ALAm\_ALAo}}}$	ALAo
	ASPm $\xrightleftharpoons{\nu_{\mathrm{ASPm\_ASPo}}}$	ASPo
	CO_2 $\xrightleftharpoons{\nu_{\mathrm{CDm\_CDo}}}$	CO_2
	FUo $\xrightleftharpoons{\nu_{\mathrm{FUo\_FUm}}}$	FUm
	GLNo $\xrightleftharpoons{\nu_{\mathrm{GLNo\_GLNm}}}$	GLNm
	GLUm $\xrightleftharpoons{\nu_{\mathrm{GLUm\_GLUo}}}$	GLUo
	ILEm $\xrightleftharpoons{\nu_{\mathrm{ILEm\_ILEo}}}$	ILEo
	IOSm $\xrightleftharpoons{\nu_{\mathrm{IOSm\_IOSo}}}$	IOSo
	LEUm $\xrightleftharpoons{\nu_{\mathrm{LEUm\_LEUo}}}$	LEUo

table continues ...

Table 2: (continued)

Gene	Reaction/flux	
	MOm $\rightleftharpoons^{\nu_{\text{MOm\_MOo}}}$	MOo
	OAo $\rightleftharpoons^{\nu_{\text{OAo\_OAm}}}$	OAm
	OGo $\rightleftharpoons^{\nu_{\text{OGo\_OGm}}}$	OGm
	ORm $\rightleftharpoons^{\nu_{\text{ORm\_ORo}}}$	ORo
	PYo $\rightleftharpoons^{\nu_{\text{PYo\_PYm}}}$	PYm
	THRo $\rightleftharpoons^{\nu_{\text{THRo\_THRm}}}$	THRm
	VALm $\rightleftharpoons^{\nu_{\text{VALm\_VALo}}}$	VALo
Mitochondrial reactions:		
	AAm $\rightleftharpoons^{\nu_{\text{AAm\_ACm}}}$	ACm
	ACm $\rightleftharpoons^{\nu_{\text{ACm\_AcCoAm}}}$	AcCoAm
	GLNm + OGm $\rightleftharpoons^{\nu_{\text{B\_GLT}}}$	2 GLUm
	GLUm $\rightleftharpoons^{\nu_{\text{B\_GLU\_OR}}}$	ORm
	HCO_3^- + OAm $\rightleftharpoons^{\nu_{\text{B\_OAm\_ASP\_01}}}$	ZvAATm
	ZvAATm $\rightleftharpoons^{\nu_{\text{B\_OAm\_ASP\_02}}}$	ASPm + YiGOGm
	OGm $\rightleftharpoons^{\nu_{\text{B\_OG\_GLU\_M}}}$	GLUm
	HCO_3^- + PYm $\rightleftharpoons^{\nu_{\text{B\_PY\_ALA\_M1}}}$	ZivALTm
	ZivALTm $\rightleftharpoons^{\nu_{\text{B\_PY\_ALA\_M2}}}$	ALAm + YiGOGm
	IOSm $\xrightarrow{\nu_{\text{B\_PY\_AcCoA\_LEU\_M}}}$	CO_2 + LEUm
	AcCoAm + MOm $\rightleftharpoons^{\nu_{\text{B\_PY\_AcCoA\_M}}}$	IOSm
	PYm $\xrightarrow{\nu_{\text{B\_PY\_M1}}}$	CO_2 + ZiiPYm
	PYm + ZiiPYm $\rightleftharpoons^{\nu_{\text{B\_PY\_M2}}}$	MOm
	THRm + ZiiPYm $\rightleftharpoons^{\nu_{\text{B\_PY\_THR\_ILE}}}$	ILEm
	MOm $\rightleftharpoons^{\nu_{\text{B\_PY\_VAL\_M}}}$	VALm
	GLUm + YiGOGm $\rightleftharpoons^{\nu_{\text{GLUm\_OGm\_01}}}$	ZviGOGm
	ZviGOGm $\rightleftharpoons^{\nu_{\text{GLUm\_OGm\_02}}}$	HCO_3^- + OGm
	CIm $\xrightarrow{\nu_{\text{TCA\_CIm\_OGm}}}$	CO_2 + OGm
	FUm $\rightleftharpoons^{\nu_{\text{TCA\_FUm\_MAm}}}$	MAm
	MAm $\rightleftharpoons^{\nu_{\text{TCA\_MAm\_OAm}}}$	OAm
	MAm $\xrightarrow{\nu_{\text{TCA\_MAm\_PYm}}}$	CO_2 + PYm
	AcCoAm + OAm $\rightleftharpoons^{\nu_{\text{TCA\_OAm\_AcCoAm\_CIm}}}$	CIm
	OGm $\xrightarrow{\nu_{\text{TCA\_OGm\_SUCoAm}}}$	CO_2 + SUCoAm
	PYm $\xrightarrow{\nu_{\text{TCA\_PYm\_AcCoAm}}}$	AcCoAm + CO_2
	SUCoAm $\rightleftharpoons^{\nu_{\text{TCA\_SUCoAm\_SUm}}}$	SUm

table continues ...

Table 2: (continued)

Gene	Reaction/flux		
	SUm	$\overset{\nu_{\text{TCA\_SUm\_FUm}}}{\rightleftharpoons}$	FUm

3 Symbolic solution of the steady state problem

3.1 Flux relations

Cytosolic flux relations:

$$\nu_{\text{AAo\_ACo}} = \nu_{\text{AcCoA}_{\text{out}}} - \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{B\_THR\_GLY}} - \nu_{\text{IOSm\_IOSo}} + \nu_{\text{LEU}_{\text{out}}} + \nu_{\text{LYS}_{\text{out}}}$$

$$\nu_{\text{ACo\_AcCoAo}} = \nu_{\text{AcCoA}_{\text{out}}} - \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{IOSm\_IOSo}} + \nu_{\text{LEU}_{\text{out}}} + \nu_{\text{LYS}_{\text{out}}} + \nu_{\text{MET}_{\text{out}}}$$

$$\nu_{\text{BCo\_CPo\_01}} = \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{BCo\_CPo\_02}} = \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{B\_AC\_01}} = \nu_{\text{MET}_{\text{out}}}$$

$$\nu_{\text{B\_ASP\_ASN}} = \nu_{\text{ASN}_{\text{out}}}$$

$$\nu_{\text{B\_ASP\_THR}} = \nu_{\text{B\_THR\_GLY}} + \nu_{\text{ILE}_{\text{out}}} + \nu_{\text{THR}_{\text{out}}}$$

$$\nu_{\text{B\_AcCoA\_01}} = \nu_{\text{MET}_{\text{out}}}$$

$$\nu_{\text{B\_GLU\_GLN}} = \nu_{\text{B\_GLT}} + \nu_{\text{GLN}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{B\_GLU\_PRO}} = \nu_{\text{PRO}_{\text{out}}}$$

$$\nu_{\text{B\_GiiiP\_GLY}} = -\nu_{\text{B\_THR\_GLY}} + \nu_{\text{GLY}_{\text{out}}}$$

$$\nu_{\text{B\_GiiiP\_SER}} = -\nu_{\text{B\_THR\_GLY}} + \nu_{\text{GLY}_{\text{out}}} + \nu_{\text{SER}_{\text{out}}} + \nu_{\text{TRP}_{\text{out}}}$$

$$\nu_{\text{B\_LYS\_C1}} = \nu_{\text{LYS}_{\text{out}}}$$

$$\nu_{\text{B\_LYS\_C2}} = \nu_{\text{LYS}_{\text{out}}}$$

$$\nu_{\text{B\_OA\_AcCoA\_MET}} = \nu_{\text{MET}_{\text{out}}}$$

$$\nu_{\text{B\_OAo\_ASP\_01}} = \nu_{\text{ASN}_{\text{out}}} + \nu_{\text{ASP}_{\text{out}}} - \nu_{\text{ASPm\_ASPo}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{ILE}_{\text{out}}} + \nu_{\text{MET}_{\text{out}}} + \nu_{\text{THR}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{B\_OAo\_ASP\_02}} = \nu_{\text{ASN}_{\text{out}}} + \nu_{\text{ASP}_{\text{out}}} - \nu_{\text{ASPm\_ASPo}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{ILE}_{\text{out}}} + \nu_{\text{MET}_{\text{out}}} + \nu_{\text{THR}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{B\_OG\_GLU\_C}} = \nu_{\text{ALA}_{\text{out}}} + \nu_{\text{ASN}_{\text{out}}} + \nu_{\text{ASP}_{\text{out}}} - \nu_{\text{ASPm\_ASPo}} - \nu_{\text{B\_PY\_ALA\_M1}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{ILE}_{\text{out}}} - \nu_{\text{LYS}_{\text{out}}} + \nu_{\text{MET}_{\text{out}}} - \nu_{\text{OGo\_OGm}} + \nu_{\text{THR}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{B\_PEP\_01}} = \nu_{\text{PHE}_{\text{out}}} + \nu_{\text{TRP}_{\text{out}}} + \nu_{\text{TYR}_{\text{out}}}$$

$$\nu_{\text{B\_PEP\_EivP\_01}} = \nu_{\text{PHE}_{\text{out}}} + \nu_{\text{TRP}_{\text{out}}} + \nu_{\text{TYR}_{\text{out}}}$$

$$\nu_{\text{B\_PEP\_EivP\_PHE}} = \nu_{\text{PHE}_{\text{out}}}$$

$$\nu_{\text{B\_PEP\_EivP\_TRP\_01}} = \nu_{\text{TRP}_{\text{out}}}$$

$$\nu_{\text{B\_PEP\_EivP\_TRP\_02}} = \nu_{\text{TRP}_{\text{out}}}$$

$$\nu_{\text{B\_PEP\_EivP\_TRP\_03}} = \nu_{\text{TRP}_{\text{out}}}$$

$\nu_{\text{B\_PEP\_EivP\_TRP\_04}} = \nu_{\text{TRP}_{\text{out}}}$

$\nu_{\text{B\_PEP\_EivP\_TRP\_05}} = \nu_{\text{TRP}_{\text{out}}}$

$\nu_{\text{B\_PEP\_EivP\_TYR}} = \nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{B\_PY\_ALA\_C1}} = \nu_{\text{ALA}_{\text{out}}} - \nu_{\text{B\_PY\_ALA\_M1}}$

$\nu_{\text{B\_PY\_ALA\_C2}} = \nu_{\text{ALA}_{\text{out}}} - \nu_{\text{B\_PY\_ALA\_M1}}$

$\nu_{\text{B\_PY\_AcCoA\_C}} = -\nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{IOSm\_IOSo}} + \nu_{\text{LEU}_{\text{out}}}$

$\nu_{\text{B\_PY\_AcCoA\_LEU\_C}} = -\nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\text{LEU}_{\text{out}}}$

$\nu_{\text{B\_PY\_VAL\_C}} = -\nu_{\text{B\_PY\_VAL\_M}} + \nu_{\text{VAL}_{\text{out}}}$

$\nu_{\text{B\_RvP\_HIS}} = \nu_{\text{HIS}_{\text{out}}}$

$\nu_{\text{CD\_BC}} = \nu_{\text{ARG}_{\text{out}}} + \nu_{\text{ASN}_{\text{out}}} + \nu_{\text{ASP}_{\text{out}}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{GLN}_{\text{out}}} + \nu_{\text{GLU}_{\text{out}}} + \nu_{\text{HIS}_{\text{out}}} + \nu_{\text{ILE}_{\text{out}}} + \nu_{\text{LYS}_{\text{out}}} + 2\nu_{\text{MET}_{\text{out}}} + \nu_{\text{OA\_PEP}} + \nu_{\text{OA}_{\text{out}}} + \nu_{\text{PRO}_{\text{out}}} + \nu_{\text{TCA\_MAm\_PYm}} + \nu_{\text{THR}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$

$\nu_{\text{FviP\_GP\_GiiiP}} = -\nu_{\text{FviP}_{\text{out}}} + \nu_{\text{GL}_{\text{in}}} - 1/3\nu_{\text{GviP\_RLvP}} - \nu_{\text{GviP}_{\text{out}}} - 2/3\nu_{\text{HIS}_{\text{out}}} - 1/3\nu_{\text{PHE}_{\text{out}}} - 2/3\nu_{\text{RvP}_{\text{out}}} - \nu_{\text{TRP}_{\text{out}}} - 1/3\nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{GLUo\_OGo\_01}} = \nu_{\text{ALA}_{\text{out}}} + \nu_{\text{ASN}_{\text{out}}} + \nu_{\text{ASP}_{\text{out}}} - \nu_{\text{ASPm\_ASPo}} - \nu_{\text{B\_PY\_ALA\_M1}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{ILE}_{\text{out}}} + \nu_{\text{MET}_{\text{out}}} + \nu_{\text{THR}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$

$\nu_{\text{GLUo\_OGo\_02}} = \nu_{\text{ALA}_{\text{out}}} + \nu_{\text{ASN}_{\text{out}}} + \nu_{\text{ASP}_{\text{out}}} - \nu_{\text{ASPm\_ASPo}} - \nu_{\text{B\_PY\_ALA\_M1}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{ILE}_{\text{out}}} + \nu_{\text{MET}_{\text{out}}} + \nu_{\text{THR}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$

$\nu_{\text{GL\_GviP}} = \nu_{\text{GL}_{\text{in}}}$

$\nu_{\text{GP\_GiiiP}} = -\nu_{\text{FviP}_{\text{out}}} + \nu_{\text{GL}_{\text{in}}} - 1/3\nu_{\text{GviP\_RLvP}} - \nu_{\text{GviP}_{\text{out}}} - 2/3\nu_{\text{HIS}_{\text{out}}} - 1/3\nu_{\text{PHE}_{\text{out}}} - 2/3\nu_{\text{RvP}_{\text{out}}} - \nu_{\text{TRP}_{\text{out}}} - 1/3\nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{GiiiP\_PEP}} = \nu_{\text{B\_THR\_GLY}} - 2\nu_{\text{FviP}_{\text{out}}} - \nu_{\text{GLY}_{\text{out}}} + 2\nu_{\text{GL}_{\text{in}}} - \nu_{\text{GiiiP}_{\text{out}}} - 1/3\nu_{\text{GviP\_RLvP}} - 2\nu_{\text{GviP}_{\text{out}}} - 5/3\nu_{\text{HIS}_{\text{out}}} - 4/3\nu_{\text{PHE}_{\text{out}}} - 5/3\nu_{\text{RvP}_{\text{out}}} - \nu_{\text{SER}_{\text{out}}} - 3\nu_{\text{TRP}_{\text{out}}} - 4/3\nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{GviP\_FviP}} = \nu_{\text{GL}_{\text{in}}} - \nu_{\text{GviP\_RLvP}} - \nu_{\text{GviP}_{\text{out}}}$

$\nu_{\text{PEP\_PY}} = \nu_{\text{B\_THR\_GLY}} - 2\nu_{\text{FviP}_{\text{out}}} - \nu_{\text{GLY}_{\text{out}}} + 2\nu_{\text{GL}_{\text{in}}} - \nu_{\text{GiiiP}_{\text{out}}} - 1/3\nu_{\text{GviP\_RLvP}} - 2\nu_{\text{GviP}_{\text{out}}} - 5/3\nu_{\text{HIS}_{\text{out}}} + \nu_{\text{OA\_PEP}} - 10/3\nu_{\text{PHE}_{\text{out}}} - 5/3\nu_{\text{RvP}_{\text{out}}} - \nu_{\text{SER}_{\text{out}}} - 5\nu_{\text{TRP}_{\text{out}}} - 10/3\nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{PPP\_FviP\_EivP\_SviiP\_GiiiP\_01}} = 1/3\nu_{\text{GviP\_RLvP}} - 1/3\nu_{\text{HIS}_{\text{out}}} + 1/3\nu_{\text{PHE}_{\text{out}}} - 1/3\nu_{\text{RvP}_{\text{out}}} + 1/3\nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{PPP\_FviP\_EivP\_SviiP\_GiiiP\_02}} = 1/3\nu_{\text{GviP\_RLvP}} - 1/3\nu_{\text{HIS}_{\text{out}}} + 1/3\nu_{\text{PHE}_{\text{out}}} - 1/3\nu_{\text{RvP}_{\text{out}}} + 1/3\nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{PPP\_FviP\_GiiiP\_XvP\_EivP\_01}} = -1/3\nu_{\text{GviP\_RLvP}} + 1/3\nu_{\text{HIS}_{\text{out}}} + 2/3\nu_{\text{PHE}_{\text{out}}} + 1/3\nu_{\text{RvP}_{\text{out}}} + \nu_{\text{TRP}_{\text{out}}} + 2/3\nu_{\text{TYR}_{\text{out}}}$

$\nu_{\text{PPP\_FviP\_GiiiP\_XvP\_EivP\_02}} = -1/3\nu_{\text{GviP\_RLvP}} + 1/3\nu_{\text{HIS}_{\text{out}}} + 2/3\nu_{\text{PHE}_{\text{out}}} + 1/3\nu_{\text{RvP}_{\text{out}}} + \nu_{\text{TRP}_{\text{out}}} + 2/3\nu_{\text{TYR}_{\text{out}}}$

$$\nu_{\text{PPP\_SviiP\_GiiiP\_XvP\_RvP\_01}} = 1/3\nu_{\text{GviP\_RLvP}} - 1/3\nu_{\text{HIS}_{\text{out}}} + 1/3\nu_{\text{PHE}_{\text{out}}} - 1/3\nu_{\text{RvP}_{\text{out}}} + 1/3\nu_{\text{TYR}_{\text{out}}}$$

$$\nu_{\text{PPP\_SviiP\_GiiiP\_XvP\_RvP\_02}} = 1/3\nu_{\text{GviP\_RLvP}} - 1/3\nu_{\text{HIS}_{\text{out}}} + 1/3\nu_{\text{PHE}_{\text{out}}} - 1/3\nu_{\text{RvP}_{\text{out}}} + 1/3\nu_{\text{TYR}_{\text{out}}}$$

$$\nu_{\text{PYo\_OAo}} = \nu_{\text{ARG}_{\text{out}}} + \nu_{\text{ASN}_{\text{out}}} + \nu_{\text{ASP}_{\text{out}}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{GLN}_{\text{out}}} + \nu_{\text{GLU}_{\text{out}}} + \nu_{\text{ILE}_{\text{out}}} + \nu_{\text{LYS}_{\text{out}}} + \nu_{\text{MET}_{\text{out}}} + \nu_{\text{OA\_PEP}} + \nu_{\text{OA}_{\text{out}}} + \nu_{\text{PRO}_{\text{out}}} + \nu_{\text{TCA\_MAm\_PYm}} + \nu_{\text{THR}_{\text{out}}}$$

$$\nu_{\text{RLvP\_RvP}} = 1/3\nu_{\text{GviP\_RLvP}} + 2/3\nu_{\text{HIS}_{\text{out}}} + 1/3\nu_{\text{PHE}_{\text{out}}} + 2/3\nu_{\text{RvP}_{\text{out}}} + \nu_{\text{TRP}_{\text{out}}} + 1/3\nu_{\text{TYR}_{\text{out}}}$$

$$\nu_{\text{US\_ARG\_OR}} = -\nu_{\text{ARG}_{\text{out}}} + \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{US\_AS\_FU\_ARG}} = \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{US\_OR\_C}} = \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{XvP\_RLvP}} = -2/3\nu_{\text{GviP\_RLvP}} + 2/3\nu_{\text{HIS}_{\text{out}}} + 1/3\nu_{\text{PHE}_{\text{out}}} + 2/3\nu_{\text{RvP}_{\text{out}}} + \nu_{\text{TRP}_{\text{out}}} + 1/3\nu_{\text{TYR}_{\text{out}}}$$

Transport relations:

$$\nu_{\text{CO}_2\text{,out}} = -3\nu_{\text{ALA}_{\text{out}}} - 6\nu_{\text{ARG}_{\text{out}}} - 4\nu_{\text{ASN}_{\text{out}}} - 4\nu_{\text{ASP}_{\text{out}}} - 2\nu_{\text{AcCoA}_{\text{out}}} - 6\nu_{\text{FviP}_{\text{out}}} - 5\nu_{\text{GLN}_{\text{out}}} - 5\nu_{\text{GLU}_{\text{out}}} - 2\nu_{\text{GLY}_{\text{out}}} + 6\nu_{\text{GL}_{\text{in}}} - 3\nu_{\text{GiiiP}_{\text{out}}} - 6\nu_{\text{GviP}_{\text{out}}} - 6\nu_{\text{HIS}_{\text{out}}} - 6\nu_{\text{ILE}_{\text{out}}} - 6\nu_{\text{LEU}_{\text{out}}} - 6\nu_{\text{LYS}_{\text{out}}} - 5\nu_{\text{MET}_{\text{out}}} - 4\nu_{\text{OA}_{\text{out}}} - 9\nu_{\text{PHE}_{\text{out}}} - 5\nu_{\text{PRO}_{\text{out}}} - 5\nu_{\text{RvP}_{\text{out}}} - 3\nu_{\text{SER}_{\text{out}}} - 4\nu_{\text{THR}_{\text{out}}} - 11\nu_{\text{TRP}_{\text{out}}} - 9\nu_{\text{TYR}_{\text{out}}} - 5\nu_{\text{VAL}_{\text{out}}}$$

Cytosolic-mitochondrial transport relations:

$$\nu_{\text{AAo\_AAm}} = -\nu_{\text{AcCoA}_{\text{out}}} + \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{IOSm\_IOSo}} - \nu_{\text{LEU}_{\text{out}}} - \nu_{\text{LYS}_{\text{out}}} + \nu_{\text{PYo\_AAo}}$$

$$\nu_{\text{ALAm\_ALAo}} = \nu_{\text{B\_PY\_ALA\_M1}}$$

$$\nu_{\text{CDm\_CDo}} = -3\nu_{\text{ALA}_{\text{out}}} - 4\nu_{\text{ARG}_{\text{out}}} - 3\nu_{\text{ASN}_{\text{out}}} - 3\nu_{\text{ASP}_{\text{out}}} - 2\nu_{\text{AcCoA}_{\text{out}}} + \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + 2\nu_{\text{B\_THR\_GLY}} - 6\nu_{\text{FviP}_{\text{out}}} - 4\nu_{\text{GLN}_{\text{out}}} - 4\nu_{\text{GLU}_{\text{out}}} - 3\nu_{\text{GLY}_{\text{out}}} + 6\nu_{\text{GL}_{\text{in}}} - 3\nu_{\text{GiiiP}_{\text{out}}} - \nu_{\text{GviP\_RLvP}} - 6\nu_{\text{GviP}_{\text{out}}} - 5\nu_{\text{HIS}_{\text{out}}} - 5\nu_{\text{ILE}_{\text{out}}} - 7\nu_{\text{LEU}_{\text{out}}} - 6\nu_{\text{LYS}_{\text{out}}} - 3\nu_{\text{MET}_{\text{out}}} - 3\nu_{\text{OA}_{\text{out}}} - 10\nu_{\text{PHE}_{\text{out}}} - 4\nu_{\text{PRO}_{\text{out}}} - \nu_{\text{PYo\_AAo}} - 5\nu_{\text{RvP}_{\text{out}}} - 3\nu_{\text{SER}_{\text{out}}} + \nu_{\text{TCA\_MAm\_PYm}} - 3\nu_{\text{THR}_{\text{out}}} - 12\nu_{\text{TRP}_{\text{out}}} - 10\nu_{\text{TYR}_{\text{out}}} - 5\nu_{\text{VAL}_{\text{out}}}$$

$$\nu_{\text{FUo\_FUm}} = \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{GLNo\_GLNm}} = \nu_{\text{B\_GLT}}$$

$$\nu_{\text{GLUm\_GLUo}} = \nu_{\text{B\_GLT}} + \nu_{\text{GLN}_{\text{out}}} + \nu_{\text{GLU}_{\text{out}}} + \nu_{\text{LYS}_{\text{out}}} + \nu_{\text{OGo\_OGm}} + \nu_{\text{PRO}_{\text{out}}}$$

$$\nu_{\text{ILEm\_ILEo}} = \nu_{\text{ILE}_{\text{out}}}$$

$$\nu_{\text{LEUm\_LEUo}} = \nu_{\text{B\_PY\_AcCoA\_LEU\_M}}$$

$$\nu_{\text{MOm\_MOo}} = -\nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{B\_PY\_VAL\_M}} - \nu_{\text{IOSm\_IOSo}} + \nu_{\text{LEU}_{\text{out}}} + \nu_{\text{VAL}_{\text{out}}}$$

$$\nu_{\text{OAo\_OAm}} = \nu_{\text{ARG}_{\text{out}}} + \nu_{\text{ASPm\_ASPo}} + \nu_{\text{GLN}_{\text{out}}} + \nu_{\text{GLU}_{\text{out}}} + \nu_{\text{LYS}_{\text{out}}} + \nu_{\text{PRO}_{\text{out}}} + \nu_{\text{TCA\_MAm\_PYm}} - \nu_{\text{US\_C\_ASP\_AS}}$$

$$\nu_{\text{ORm\_ORo}} = \nu_{\text{ARG}_{\text{out}}}$$

$$\nu_{\text{PYo\_PYm}} = -\nu_{\text{ALA}_{\text{out}}} - \nu_{\text{ARG}_{\text{out}}} - \nu_{\text{ASN}_{\text{out}}} - \nu_{\text{ASP}_{\text{out}}} + \nu_{\text{B\_PY\_ALA\_M1}} - 2\nu_{\text{FviP}_{\text{out}}} - \nu_{\text{GLN}_{\text{out}}} -$$

$\nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - \nu_{\mathrm{ILE_{out}}} - \nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - \nu_{\mathrm{PRO_{out}}} - \nu_{\mathrm{PYo\_AAo}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{TCA\_MAm\_PYm}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}}$

$\nu_{\mathrm{THRo\_THRm}} = \nu_{\mathrm{ILE_{out}}}$

$\nu_{\mathrm{VALm\_VALo}} = \nu_{\mathrm{B\_PY\_VAL\_M}}$

Mitochondrial flux relations:

$\nu_{\mathrm{AAm\_ACm}} = -\nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\mathrm{B\_THR\_GLY}} + \nu_{\mathrm{IOSm\_IOSo}} - \nu_{\mathrm{LEU_{out}}} - \nu_{\mathrm{LYS_{out}}} + \nu_{\mathrm{PYo\_AAo}}$

$\nu_{\mathrm{ACm\_AcCoAm}} = -\nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\mathrm{B\_THR\_GLY}} + \nu_{\mathrm{IOSm\_IOSo}} - \nu_{\mathrm{LEU_{out}}} - \nu_{\mathrm{LYS_{out}}} + \nu_{\mathrm{PYo\_AAo}}$

$\nu_{\mathrm{B\_GLU\_OR}} = \nu_{\mathrm{ARG_{out}}}$

$\nu_{\mathrm{B\_OAm\_ASP\_01}} = \nu_{\mathrm{ASPm\_ASPo}}$

$\nu_{\mathrm{B\_OAm\_ASP\_02}} = \nu_{\mathrm{ASPm\_ASPo}}$

$\nu_{\mathrm{B\_OG\_GLU\_M}} = \nu_{\mathrm{ARG_{out}}} + \nu_{\mathrm{ASPm\_ASPo}} - \nu_{\mathrm{B\_GLT}} + \nu_{\mathrm{B\_PY\_ALA\_M1}} + \nu_{\mathrm{GLN_{out}}} + \nu_{\mathrm{GLU_{out}}} + \nu_{\mathrm{LYS_{out}}} + \nu_{\mathrm{OGo\_OGm}} + \nu_{\mathrm{PRO_{out}}}$

$\nu_{\mathrm{B\_PY\_ALA\_M2}} = \nu_{\mathrm{B\_PY\_ALA\_M1}}$

$\nu_{\mathrm{B\_PY\_AcCoA\_M}} = \nu_{\mathrm{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\mathrm{IOSm\_IOSo}}$

$\nu_{\mathrm{B\_PY\_M1}} = \nu_{\mathrm{ILE_{out}}} + \nu_{\mathrm{LEU_{out}}} + \nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{B\_PY\_M2}} = \nu_{\mathrm{LEU_{out}}} + \nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{B\_PY\_THR\_ILE}} = \nu_{\mathrm{ILE_{out}}}$

$\nu_{\mathrm{GLUm\_OGm\_01}} = \nu_{\mathrm{ASPm\_ASPo}} + \nu_{\mathrm{B\_PY\_ALA\_M1}}$

$\nu_{\mathrm{GLUm\_OGm\_02}} = \nu_{\mathrm{ASPm\_ASPo}} + \nu_{\mathrm{B\_PY\_ALA\_M1}}$

$\nu_{\mathrm{TCA\_CIm\_OGm}} = -\nu_{\mathrm{ALA_{out}}} - \nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - \nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_THR\_GLY}} - 2\nu_{\mathrm{FviP_{out}}} - \nu_{\mathrm{GLN_{out}}} - \nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 3\nu_{\mathrm{LEU_{out}}} - 2\nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - \nu_{\mathrm{PRO_{out}}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} - 2\nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{TCA\_FUm\_MAm}} = -\nu_{\mathrm{ALA_{out}}} - 2\nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - \nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_THR\_GLY}} - 2\nu_{\mathrm{FviP_{out}}} - 2\nu_{\mathrm{GLN_{out}}} - 2\nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 3\nu_{\mathrm{LEU_{out}}} - 3\nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - 2\nu_{\mathrm{PRO_{out}}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} + \nu_{\mathrm{US\_C\_ASP\_AS}} - 2\nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{TCA\_MAm\_OAm}} = -\nu_{\mathrm{ALA_{out}}} - 2\nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - \nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_THR\_GLY}} - 2\nu_{\mathrm{FviP_{out}}} - 2\nu_{\mathrm{GLN_{out}}} - 2\nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 3\nu_{\mathrm{LEU_{out}}} - 3\nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - 2\nu_{\mathrm{PRO_{out}}} -$

$5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{TCA\_MAm\_PYm}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} + \nu_{\mathrm{US\_C\_ASP\_AS}} - 2\nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{TCA\_OAm\_AcCoAm\_CIm}} = -\nu_{\mathrm{ALA_{out}}} - \nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - \nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_THR\_GLY}} - 2\nu_{\mathrm{FviP_{out}}} - \nu_{\mathrm{GLN_{out}}} - \nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 3\nu_{\mathrm{LEU_{out}}} - 2\nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - \nu_{\mathrm{PRO_{out}}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} - 2\nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{TCA\_OGm\_SUCoAm}} = -\nu_{\mathrm{ALA_{out}}} - 2\nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - \nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_THR\_GLY}} - 2\nu_{\mathrm{FviP_{out}}} - 2\nu_{\mathrm{GLN_{out}}} - 2\nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 3\nu_{\mathrm{LEU_{out}}} - 3\nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - 2\nu_{\mathrm{PRO_{out}}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} - 2\nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{TCA\_PYm\_AcCoAm}} = -\nu_{\mathrm{ALA_{out}}} - \nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - 2\nu_{\mathrm{FviP_{out}}} - \nu_{\mathrm{GLN_{out}}} - \nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 2\nu_{\mathrm{LEU_{out}}} - \nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - \nu_{\mathrm{PRO_{out}}} - \nu_{\mathrm{PYo\_AAo}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} - 2\nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{TCA\_SUCoAm\_SUm}} = -\nu_{\mathrm{ALA_{out}}} - 2\nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - \nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_THR\_GLY}} - 2\nu_{\mathrm{FviP_{out}}} - 2\nu_{\mathrm{GLN_{out}}} - 2\nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 3\nu_{\mathrm{LEU_{out}}} - 3\nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - 2\nu_{\mathrm{PRO_{out}}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} - 2\nu_{\mathrm{VAL_{out}}}$

$\nu_{\mathrm{TCA\_SUm\_FUm}} = -\nu_{\mathrm{ALA_{out}}} - 2\nu_{\mathrm{ARG_{out}}} - \nu_{\mathrm{ASN_{out}}} - \nu_{\mathrm{ASP_{out}}} - \nu_{\mathrm{AcCoA_{out}}} + \nu_{\mathrm{B\_THR\_GLY}} - 2\nu_{\mathrm{FviP_{out}}} - 2\nu_{\mathrm{GLN_{out}}} - 2\nu_{\mathrm{GLU_{out}}} - \nu_{\mathrm{GLY_{out}}} + 2\nu_{\mathrm{GL_{in}}} - \nu_{\mathrm{GiiiP_{out}}} - 1/3\nu_{\mathrm{GviP\_RLvP}} - 2\nu_{\mathrm{GviP_{out}}} - 5/3\nu_{\mathrm{HIS_{out}}} - 2\nu_{\mathrm{ILE_{out}}} - 3\nu_{\mathrm{LEU_{out}}} - 3\nu_{\mathrm{LYS_{out}}} - \nu_{\mathrm{MET_{out}}} - \nu_{\mathrm{OA_{out}}} - 10/3\nu_{\mathrm{PHE_{out}}} - 2\nu_{\mathrm{PRO_{out}}} - 5/3\nu_{\mathrm{RvP_{out}}} - \nu_{\mathrm{SER_{out}}} - \nu_{\mathrm{THR_{out}}} - 4\nu_{\mathrm{TRP_{out}}} - 10/3\nu_{\mathrm{TYR_{out}}} - 2\nu_{\mathrm{VAL_{out}}}$

3.2 Constraints

The following constraints are implications of irreversibility conditions (positiveness of unidirectional fluxes) in the system of reactions:

$3\nu_{\mathrm{ALA_{out}}} + 3\nu_{\mathrm{ARG_{out}}} + 3\nu_{\mathrm{ASN_{out}}} + 3\nu_{\mathrm{ASP_{out}}} + 6\nu_{\mathrm{FviP_{out}}} + 3\nu_{\mathrm{GLN_{out}}} + 3\nu_{\mathrm{GLU_{out}}} + 3\nu_{\mathrm{GLY_{out}}} + 3\nu_{\mathrm{GiiiP_{out}}} + \nu_{\mathrm{GviP\_RLvP}} + 6\nu_{\mathrm{GviP_{out}}} + 5\nu_{\mathrm{HIS_{out}}} + 6\nu_{\mathrm{ILE_{out}}} + 6\nu_{\mathrm{LEU_{out}}} + 3\nu_{\mathrm{LYS_{out}}} + 3\nu_{\mathrm{MET_{out}}} + 3\nu_{\mathrm{OA_{out}}} + 10\nu_{\mathrm{PHE_{out}}} + 3\nu_{\mathrm{PRO_{out}}} + 3\nu_{\mathrm{PYo\_AAo}} + 5\nu_{\mathrm{RvP_{out}}} + 3\nu_{\mathrm{SER_{out}}} + 3\nu_{\mathrm{THR_{out}}} + 12\nu_{\mathrm{TRP_{out}}} + 10\nu_{\mathrm{TYR_{out}}} + 6\nu_{\mathrm{VAL_{out}}} \leq 6\nu_{\mathrm{GL_{in}}}$

$3\nu_{\mathrm{ALA_{out}}} + 6\nu_{\mathrm{ARG_{out}}} + 3\nu_{\mathrm{ASN_{out}}} + 3\nu_{\mathrm{ASP_{out}}} + 3\nu_{\mathrm{AcCoA_{out}}} + 6\nu_{\mathrm{FviP_{out}}} + 6\nu_{\mathrm{GLN_{out}}} + 6\nu_{\mathrm{GLU_{out}}} + 3\nu_{\mathrm{GLY_{out}}} + 3\nu_{\mathrm{GiiiP_{out}}} + \nu_{\mathrm{GviP\_RLvP}} + 6\nu_{\mathrm{GviP_{out}}} + 5\nu_{\mathrm{HIS_{out}}} + 6\nu_{\mathrm{ILE_{out}}} + 9\nu_{\mathrm{LEU_{out}}} + 9\nu_{\mathrm{LYS_{out}}} + 3\nu_{\mathrm{MET_{out}}} + 3\nu_{\mathrm{OA_{out}}} + 10\nu_{\mathrm{PHE_{out}}} + 6\nu_{\mathrm{PRO_{out}}} + 5\nu_{\mathrm{RvP_{out}}} + 3\nu_{\mathrm{SER_{out}}} + 3\nu_{\mathrm{THR_{out}}} + 12\nu_{\mathrm{TRP_{out}}} + 10\nu_{\mathrm{TYR_{out}}} + 6\nu_{\mathrm{VAL_{out}}} \leq 3\nu_{\mathrm{B\_THR\_GLY}} + 6\nu_{\mathrm{GL_{in}}}$

$3/2\nu_{\mathrm{ALA_{out}}} + 3\nu_{\mathrm{ARG_{out}}} + 2\nu_{\mathrm{ASN_{out}}} + 2\nu_{\mathrm{ASP_{out}}} + \nu_{\mathrm{AcCoA_{out}}} + 3\nu_{\mathrm{FviP_{out}}} + 5/2\nu_{\mathrm{GLN_{out}}} + 5/2\nu_{\mathrm{GLU_{out}}} + \nu_{\mathrm{GLY_{out}}} + 3/2\nu_{\mathrm{GiiiP_{out}}} + 3\nu_{\mathrm{GviP_{out}}} + 3\nu_{\mathrm{HIS_{out}}} + 3\nu_{\mathrm{ILE_{out}}} + 3\nu_{\mathrm{LEU_{out}}} + 3\nu_{\mathrm{LYS_{out}}} + 5/2\nu_{\mathrm{MET_{out}}} + 2\nu_{\mathrm{OA_{out}}} + 9/2\nu_{\mathrm{PHE_{out}}} + 5/2\nu_{\mathrm{PRO_{out}}} + 5/2\nu_{\mathrm{RvP_{out}}} + 3/2\nu_{\mathrm{SER_{out}}} + 2\nu_{\mathrm{THR_{out}}} + 11/2\nu_{\mathrm{TRP_{out}}} + 9/2\nu_{\mathrm{TYR_{out}}} + 5/2\nu_{\mathrm{VAL_{out}}} \leq 3\nu_{\mathrm{GL_{in}}}$

$\nu_{\mathrm{ARG_{out}}} \leq \nu_{\mathrm{US\_C\_ASP\_AS}}$

$\nu_{\mathrm{B\_PY\_AcCoA\_LEU\_M}} \leq \nu_{\mathrm{LEU_{out}}}$

$\nu_{\mathrm{B\_THR\_GLY}} \leq \nu_{\mathrm{GLY_{out}}}$

4 Values of independent fluxes used to generate Figure 1.

External flux	Value (a.u.)	Internal flux	Value (a.u.)
$\nu_{\mathrm{ALA_{out}}}$	2.77	$\nu_{\mathrm{ASPm\_ASPo}}$	2
$\nu_{\mathrm{ARG_{out}}}$	1.94	$\nu_{\mathrm{B\_GLT}}$	4
$\nu_{\mathrm{ASN_{out}}}$	0.82	$\nu_{\mathrm{B\_PY\_ALA\_M1}}$	1.0
$\nu_{\mathrm{ASP_{out}}}$	2.39	$\nu_{\mathrm{B\_PY\_AcCoA\_LEU\_M}}$	2
$\nu_{\mathrm{AcCoA_{out}}}$	0.3	$\nu_{\mathrm{B\_PY\_VAL\_M}}$	1
$\nu_{\mathrm{FviP_{out}}}$	11	$\nu_{\mathrm{B\_THR\_GLY}}$	0
$\nu_{\mathrm{GLN_{out}}}$	1.06	$\nu_{\mathrm{GviP\_RLvP}}$	5
$\nu_{\mathrm{GLU_{out}}}$	3.04	$\nu_{\mathrm{IOSm\_IOSo}}$	0
$\nu_{\mathrm{GLY_{out}}}$	1.17	$\nu_{\mathrm{OA\_PEP}}$	0
$\nu_{\mathrm{GL_{in}}}$	100	$\nu_{\mathrm{OGo\_OGm}}$	0
$\nu_{\mathrm{GiiiP_{out}}}$	0.45	$\nu_{\mathrm{PYo\_AAo}}$	10
$\nu_{\mathrm{GviP_{out}}}$	3.8	$\nu_{\mathrm{TCA\_MAm\_PYm}}$	0
$\nu_{\mathrm{HIS_{out}}}$	0.8	$\nu_{\mathrm{US\_C\_ASP\_AS}}$	2.5
$\nu_{\mathrm{ILE_{out}}}$	2.33		
$\nu_{\mathrm{LEU_{out}}}$	3.57		
$\nu_{\mathrm{LYS_{out}}}$	3.45		
$\nu_{\mathrm{MET_{out}}}$	0.51		
$\nu_{\mathrm{OA_{out}}}$	0.36		
$\nu_{\mathrm{PHE_{out}}}$	2.43		
$\nu_{\mathrm{PRO_{out}}}$	1.66		
$\nu_{\mathrm{RvP_{out}}}$	2.6		
$\nu_{\mathrm{SER_{out}}}$	1.12		
$\nu_{\mathrm{THR_{out}}}$	1.54		
$\nu_{\mathrm{TRP_{out}}}$	0.62		
$\nu_{\mathrm{TYR_{out}}}$	1.84		
$\nu_{\mathrm{VAL_{out}}}$	2.66		

5 Symbolic solution of the steady state problem with measured values

5.1 Flux relations

Final flux values after substituting all specified independent flux values from the above Table are shown in bold.

Cytosolic flux relations:

$\nu_{\text{AAo\_ACo}} = 7.320 - \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{B\_THR\_GLY}} - \nu_{\text{IOSm\_IOSo}} = \mathbf{5.320}$

$\nu_{\text{ACo\_AcCoAo}} = 7.830 - \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{IOSm\_IOSo}} = \mathbf{5.830}$

$\nu_{\text{BCo\_CPo\_01}} = \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{2.500}$

$\nu_{\text{BCo\_CPo\_02}} = \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{2.500}$

$\nu_{\text{B\_AC\_01}} = 0.510 = \mathbf{0.510}$

$\nu_{\text{B\_ASP\_ASN}} = 0.820 = \mathbf{0.820}$

$\nu_{\text{B\_ASP\_THR}} = 3.870 + \nu_{\text{B\_THR\_GLY}} = \mathbf{3.870}$

$\nu_{\text{B\_AcCoA\_01}} = 0.510 = \mathbf{0.510}$

$\nu_{\text{B\_GLU\_GLN}} = 1.060 + \nu_{\text{B\_GLT}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{7.560}$

$\nu_{\text{B\_GLU\_PRO}} = 1.660 = \mathbf{1.660}$

$\nu_{\text{B\_GiiiP\_GLY}} = 1.170 - \nu_{\text{B\_THR\_GLY}} = \mathbf{1.170}$

$\nu_{\text{B\_GiiiP\_SER}} = 2.910 - \nu_{\text{B\_THR\_GLY}} = \mathbf{2.910}$

$\nu_{\text{B\_LYS\_C1}} = 3.450 = \mathbf{3.450}$

$\nu_{\text{B\_LYS\_C2}} = 3.450 = \mathbf{3.450}$

$\nu_{\text{B\_OA\_AcCoA\_MET}} = 0.510 = \mathbf{0.510}$

$\nu_{\text{B\_OAo\_ASP\_01}} = 7.590 - \nu_{\text{ASPm\_ASPo}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{8.090}$

$\nu_{\text{B\_OAo\_ASP\_02}} = 7.590 - \nu_{\text{ASPm\_ASPo}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{8.090}$

$\nu_{\text{B\_OG\_GLU\_C}} = 6.910 - \nu_{\text{ASPm\_ASPo}} - \nu_{\text{B\_PY\_ALA\_M1}} + \nu_{\text{B\_THR\_GLY}} - \nu_{\text{OGo\_OGm}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{6.410}$

$\nu_{\text{B\_PEP\_01}} = 4.890 = \mathbf{4.890}$

$\nu_{\text{B\_PEP\_EivP\_01}} = 4.890 = \mathbf{4.890}$

$\nu_{\text{B\_PEP\_EivP\_PHE}} = 2.430 = \mathbf{2.430}$

$\nu_{\text{B\_PEP\_EivP\_TRP\_01}} = 0.620 = \mathbf{0.620}$

$\nu_{\text{B\_PEP\_EivP\_TRP\_02}} = 0.620 = \mathbf{0.620}$

$\nu_{\text{B\_PEP\_EivP\_TRP\_03}} = 0.620 = \mathbf{0.620}$

$\nu_{\text{B\_PEP\_EivP\_TRP\_04}} = 0.620 = \mathbf{0.620}$

$\nu_{\text{B\_PEP\_EivP\_TRP\_05}} = 0.620 = \mathbf{0.620}$

$\nu_{\text{B\_PEP\_EivP\_TYR}} = 1.840 = \mathbf{1.840}$

$\nu_{\text{B\_PY\_ALA\_C1}} = 2.770 - \nu_{\text{B\_PY\_ALA\_M1}} = \mathbf{1.770}$

$\nu_{\text{B\_PY\_ALA\_C2}} = 2.770 - \nu_{\text{B\_PY\_ALA\_M1}} = \mathbf{1.770}$

$\nu_{\text{B\_PY\_AcCoA\_C}} = 3.570 - \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{IOSm\_IOSo}} = \mathbf{1.570}$

$\nu_{\text{B\_PY\_AcCoA\_LEU\_C}} = 3.570 - \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} = \mathbf{1.570}$

$\nu_{\text{B\_PY\_VAL\_C}} = 2.660 - \nu_{\text{B\_PY\_VAL\_M}} = \mathbf{1.660}$

$\nu_{\text{B\_RvP\_HIS}} = 0.800 = \mathbf{0.800}$

$\nu_{\text{CD\_BC}} = 20.410 + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{OA\_PEP}} + \nu_{\text{TCA\_MAm\_PYm}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{22.910}$

$\nu_{\text{FviP\_GP\_GiiiP}} = 80.890 - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{79.223}$

$\nu_{\text{GLUo\_OGo\_01}} = 10.360 - \nu_{\text{ASPm\_ASPo}} - \nu_{\text{B\_PY\_ALA\_M1}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{9.860}$

$\nu_{\text{GLUo\_OGo\_02}} = 10.360 - \nu_{\text{ASPm\_ASPo}} - \nu_{\text{B\_PY\_ALA\_M1}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{9.860}$

$\nu_{\text{GL\_GviP}} = 100.000 = \mathbf{100.000}$

$\nu_{\text{GP\_GiiiP}} = 80.890 - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{79.223}$

$\nu_{\text{GiiiP\_PEP}} = 154.440 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{152.773}$

$\nu_{\text{GviP\_FviP}} = 96.200 - \nu_{\text{GviP\_RLvP}} = \mathbf{91.200}$

$\nu_{\text{PEP\_PY}} = 144.660 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} + \nu_{\text{OA\_PEP}} = \mathbf{142.993}$

$\nu_{\text{PPP\_FviP\_EivP\_SviiP\_GiiiP\_01}} = 0.290 + 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{1.957}$

$\nu_{\text{PPP\_FviP\_EivP\_SviiP\_GiiiP\_02}} = 0.290 + 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{1.957}$

$\nu_{\text{PPP\_FviP\_GiiiP\_XvP\_EivP\_01}} = 4.600 - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{2.933}$

$\nu_{\text{PPP\_FviP\_GiiiP\_XvP\_EivP\_02}} = 4.600 - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{2.933}$

$\nu_{\text{PPP\_SviiP\_GiiiP\_XvP\_RvP\_01}} = 0.290 + 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{1.957}$

$\nu_{\text{PPP\_SviiP\_GiiiP\_XvP\_RvP\_02}} = 0.290 + 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{1.957}$

$\nu_{\text{PYo\_OAo}} = 19.100 + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{OA\_PEP}} + \nu_{\text{TCA\_MAm\_PYm}} = \mathbf{19.100}$

$\nu_{\text{RLvP\_RvP}} = 4.310 + 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{5.977}$

$\nu_{\text{US\_ARG\_OR}} = -1.940 + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{0.560}$

$\nu_{\text{US\_AS\_FU\_ARG}} = \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{2.500}$

$\nu_{\text{US\_OR\_C}} = \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{2.500}$

$\nu_{\text{XvP\_RLvP}} = 4.310 - 2/3\nu_{\text{GviP\_RLvP}} = \mathbf{0.977}$

Transport relations:

$\nu_{\text{CO}_2\text{,out}} = 299.360 = \mathbf{299.360}$

Cytosolic-mitochondrial transport relations:

$\nu_{\text{AAo\_AAm}} = -7.320 + \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{IOSm\_IOSo}} + \nu_{\text{PYo\_AAo}} = \mathbf{4.680}$

$\nu_{\text{ALAm\_ALAo}} = \nu_{\text{B\_PY\_ALA\_M1}} = \mathbf{1.000}$

$\nu_{\text{CDm\_CDo}} = 308.630 + \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + 2\nu_{\text{B\_THR\_GLY}} - \nu_{\text{GviP\_RLvP}} - \nu_{\text{PYo\_AAo}} + \nu_{\text{TCA\_MAm\_PYm}} = \mathbf{295.630}$

$\nu_{\text{FUo\_FUm}} = \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{2.500}$

$\nu_{\text{GLNo\_GLNm}} = \nu_{\text{B\_GLT}} = \mathbf{4.000}$

$\nu_{\text{GLUm\_GLUo}} = 9.210 + \nu_{\text{B\_GLT}} + \nu_{\text{OGo\_OGm}} = \mathbf{13.210}$

$\nu_{\text{ILEm\_ILEo}} = 2.330 = \mathbf{2.330}$

$\nu_{\text{LEUm\_LEUo}} = \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} = \mathbf{2.000}$

$\nu_{\text{MOm\_MOo}} = 6.230 - \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} - \nu_{\text{B\_PY\_VAL\_M}} - \nu_{\text{IOSm\_IOSo}} = \mathbf{3.230}$

$\nu_{\text{OAo\_OAm}} = 11.150 + \nu_{\text{ASPm\_ASPo}} + \nu_{\text{TCA\_MAm\_PYm}} - \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{10.650}$

$\nu_{\text{ORm\_ORo}} = 1.940 = \mathbf{1.940}$

$\nu_{\text{PYo\_PYm}} = 123.410 + \nu_{\text{B\_PY\_ALA\_M1}} - 1/3\nu_{\text{GviP\_RLvP}} - \nu_{\text{PYo\_AAo}} - \nu_{\text{TCA\_MAm\_PYm}} = \mathbf{112.743}$

$\nu_{\text{THRo\_THRm}} = 2.330 = \mathbf{2.330}$

$\nu_{\text{VALm\_VALo}} = \nu_{\text{B\_PY\_VAL\_M}} = \mathbf{1.000}$

Mitochondrial flux relations:

$\nu_{\text{AAm\_ACm}} = -7.320 + \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{IOSm\_IOSo}} + \nu_{\text{PYo\_AAo}} = \mathbf{4.680}$

$\nu_{\text{ACm\_AcCoAm}} = -7.320 + \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\text{B\_THR\_GLY}} + \nu_{\text{IOSm\_IOSo}} + \nu_{\text{PYo\_AAo}} = \mathbf{4.680}$

$\nu_{\text{B\_GLU\_OR}} = 1.940 = \mathbf{1.940}$

$\nu_{\text{B\_OAm\_ASP\_01}} = \nu_{\text{ASPm\_ASPo}} = \mathbf{2.000}$

$\nu_{\text{B\_OAm\_ASP\_02}} = \nu_{\text{ASPm\_ASPo}} = \mathbf{2.000}$

$\nu_{\text{B\_OG\_GLU\_M}} = 11.150 + \nu_{\text{ASPm\_ASPo}} - \nu_{\text{B\_GLT}} + \nu_{\text{B\_PY\_ALA\_M1}} + \nu_{\text{OGo\_OGm}} = \mathbf{10.150}$

$\nu_{\text{B\_PY\_ALA\_M2}} = \nu_{\text{B\_PY\_ALA\_M1}} = \mathbf{1.000}$

$\nu_{\text{B\_PY\_AcCoA\_M}} = \nu_{\text{B\_PY\_AcCoA\_LEU\_M}} + \nu_{\text{IOSm\_IOSo}} = \mathbf{2.000}$

$\nu_{\text{B\_PY\_M1}} = 8.560 = \mathbf{8.560}$

$\nu_{\text{B\_PY\_M2}} = 6.230 = \mathbf{6.230}$

$\nu_{\text{B\_PY\_THR\_ILE}} = 2.330 = \mathbf{2.330}$

$\nu_{\text{GLUm\_OGm\_01}} = \nu_{\text{ASPm\_ASPo}} + \nu_{\text{B\_PY\_ALA\_M1}} = \mathbf{3.000}$

$\nu_{\text{GLUm\_OGm\_02}} = \nu_{\text{ASPm\_ASPo}} + \nu_{\text{B\_PY\_ALA\_M1}} = \mathbf{3.000}$

$\nu_{\text{TCA\_CIm\_OGm}} = 101.300 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{99.633}$

$\nu_{\text{TCA\_FUm\_MAm}} = 90.150 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{90.983}$

$\nu_{\text{TCA\_MAm\_OAm}} = 90.150 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} - \nu_{\text{TCA\_MAm\_PYm}} + \nu_{\text{US\_C\_ASP\_AS}} = \mathbf{90.983}$

$\nu_{\text{TCA\_OAm\_AcCoAm\_CIm}} = 101.300 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{99.633}$

$\nu_{\text{TCA\_OGm\_SUCoAm}} = 90.150 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{88.483}$

$\nu_{\text{TCA\_PYm\_AcCoAm}} = 108.620 - 1/3\nu_{\text{GviP\_RLvP}} - \nu_{\text{PYo\_AAo}} = \mathbf{96.953}$

$\nu_{\text{TCA\_SUCoAm\_SUm}} = 90.150 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{88.483}$

$\nu_{\text{TCA\_SUm\_FUm}} = 90.150 + \nu_{\text{B\_THR\_GLY}} - 1/3\nu_{\text{GviP\_RLvP}} = \mathbf{88.483}$

5.2 Constraints

$1.94 \leq \nu_{\text{US\_C\_ASP\_AS}}$

$\nu_{\text{B\_PY\_AcCoA\_LEU\_M}} \leq 3.57$

$\nu_{\text{B\_THR\_GLY}} \leq 1.17$

$\nu_{\text{GviP\_RLvP}} + 3.0\nu_{\text{PYo\_AAo}} \leq 325.86$

$\nu_{\text{GviP\_RLvP}} \leq 270.45 + 3.0\nu_{\text{B\_THR\_GLY}}$

Table 3: Extreme independent fluxes

Fluxes	1	2	3	4	5	6	7	8	9	10	11	12
$\nu_{\text{ASPm\_ASPo}}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$\nu_{\text{B\_GLT}}$	-70.15	21.17	21.17	-70.15	21.17	21.17	21.17	21.17	-70.15	21.17	21.17	-70.15
$\nu_{\text{B\_PY\_ALA\_M1}}$	2.77	2.77	2.77	2.77	2.77	2.77	2.77	2.77	2.77	2.77	2.77	2.77
$\nu_{\text{B\_PY\_AcCoA\_LEU\_M}}$	3.57	3.57	3.57	3.57	3.57	3.57	0.0	0.0	0.0	0.0	0.0	0.0
$\nu_{\text{B\_PY\_VAL\_M}}$	2.66	2.66	2.66	2.66	2.66	2.66	2.66	2.66	2.66	2.66	2.66	2.66
$\nu_{\text{B\_THR\_GLY}}$	-90.15	1.17	1.17	-90.15	1.17	1.17	1.17	1.17	-90.15	1.17	1.17	-90.15
$\nu_{\text{GviP\_RLvP}}$	0.0	0.0	0.0	0.0	273.96	273.96	273.96	273.96	0.0	0.0	0.0	0.0
$\nu_{\text{IOSm\_IOSo}}$	93.9	2.58	-106.04	-14.72	-14.72	2.58	-11.15	6.15	-11.15	-102.47	6.15	97.47
$\nu_{\text{OA\_PEP}}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$\nu_{\text{OGo\_OGm}}$	-84.07	7.25	7.25	-84.07	7.25	7.25	7.25	7.25	-84.07	7.25	7.25	-84.07
$\nu_{\text{PYo\_AAo}}$	0.0	0.0	108.62	108.62	17.3	0.0	17.3	0.0	108.62	108.62	0.0	0.0
$\nu_{\text{TCA\_MAm\_PYm}}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$\nu_{\text{US\_C\_ASP\_AS}}$	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94	1.94