# Definition of the simulations and solution summary

## Contents

# 1 Definitions and specification of exchange sets

**List of compartments**

| Identifer | compartment | comment |
|---|---|---|
| s | sinusoid (blood) | external |
| b | bile | external |
| c | cytosol | |
| m | mitochondrium | |
| r | ER and Golgi | combined |
| p | peroxysome | |
| l | lysosome | |
| n | nucleus | |

**Symbols in *Constraints* column**

| Symbol | meaning |
|---|---|
| $-$ | uptake allowed |
| $+$ | excretion allowed |
| $=$ | any exchange allowed |
| MCES/AAA/ALFA/PIPES | use exchange set (see below) |

**Maintained cell exchange set: MCES**

| Metabolite | compartment | direction |
|---|---|---|
| ATP-energy | c | both |
| ATP-energy | m | both |
| Activated methyl group | c | both |
| THF-activated methyl group | c | both |
| NADH-redox-potential | r | both |
| NADH-redox-potential | c | both |
| NADH-redox-potential | m | both |
| NADH-redox-potential | p | both |
| NADPH-redox-potential | r | both |
| NADPH-redox-potential | c | both |
| NADPH-redox-potential | m | both |
| NADPH-redox-potential | p | both |
| FADH-redox-potential | c | both |
| Adenosylmethioninamine-potential | c | both |
| Proton-gradient | c | both |
| Proton-gradient | m | both |
| activated-sulphur | c | both |
| Glucose-6P | c | both |
| Pyruvate | c | both |
| Pyruvate | m | both |
| Farnesyl-PP | r | both |
| Farnesyl-PP | p | both |
| CoA-activated acetyl group | c | both |
| CoA-activated acetyl group | m | both |
| CoA-activated acetyl group | p | both |
| CoA-activated acetyl group | r | both |
| Na-gradient | c | both |
| $P_i$ | c | both |
| $H_2O$ | s | both |
| $CO_2$ | s | export |
| $O_2$ | s | import |

**All amino acids: AAA**

| Metabolite | compartment | direction |
|---|---|---|
| Histidine | s | both |
| Isoleucine | s | both |
| Leucine | s | both |
| Lysine | s | both |
| Methionine | s | both |
| Phenylalanine | s | both |
| Threonine | s | both |
| Tryptophan | s | both |
| Valine | s | both |
| Alanine | s | both |
| Arginine | s | both |
| Asparagine | s | both |
| Aspartate | s | both |
| Cysteine | s | both |
| Cystine | s | both |
| Glutamate | s | both |
| Glycine | s | both |
| Glutamine | s | both |
| Proline | s | both |
| Serine | s | both |
| Tyrosine | s | both |

**All lipid-relevant fatty acids and group donors: ALFA**

| Metabolite | compartment | direction |
|---|---|---|
| Linoleate | c | both |
| Palmitate | c | both |
| Stearate | c | both |
| Oleate | c | both |
| Arachidonate | c | both |
| Palmitolate | c | both |
| gamma-Linolenate | c | both |
| Ethanolamine | c | both |
| Choline | c | both |

**Physiological exchange set: PIPES**

| Metabolite | compartment | direction |
|---|---|---|
| Glucose | s | both |
| $O_2$ | s | import |
| $NH_3$ | s | import |
| Sulfate | s | both |
| $P_i$ | s | both |
| $Fe^{2+}$ | s | both |
| Nicotinamide | s | import |
| Folate | s | import |
| Histidine | s | both |
| Isoleucine | s | both |
| Leucine | s | both |
| Lysine | s | both |
| Methionine | s | both |
| Phenylalanine | s | both |
| Threonine | s | both |
| Tryptophan | s | both |
| Valine | s | both |
| Pantothenate | s | import |
| $CO_2$ | s | export |
| Urea | s | export |
| Urate | s | export |
| Ethanolamine | c | both |
| Choline | c | both |
| Linoleate | s | both |
| Pyridoxine | s | import |
| Riboflavin | s | import |
| $H_2O$ | s | both |
| L-Lactate | s | both |
| Alanine | s | both |
| Arginine | s | both |
| Asparagine | s | both |
| Aspartate | s | both |
| Cysteine | s | both |
| Cystine | s | both |
| Glutamate | s | both |
| Glycine | s | both |
| Glutamine | s | both |
| Proline | s | both |
| Serine | s | both |
| Tyrosine | s | both |
| Palmitate | s | both |
| Stearate | s | both |
| Oleate | s | both |
| Arachidonate | s | both |
| Palmitolate | s | both |
| Cholesterol | b | export |
| $H_2S$ | s | export |

# 2 A. Maintenance functions

## 2.1 A1. pure energy

Table 1: A1. pure energy

| Simulation | | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| **A1.1. NTP rephosphorylation** | | | | | | | | | | | | | | | | | | | |
| 1 | Aerobic ATP rephosph (FA) | ATP-energy(c) | −Palmitate +$CO_2$ −$O_2$ =$H_2O$ | Aerobic rephosphorylation of cytosolic ATP from a fatty acid | 0.22 $O_2$(s) 0.01 Palmitate(s) | 0.15 $H_2O$(s) 0.15 $CO_2$(s) 1 ATP-energy(c) | 6 | 38 | - | - | - | - | - | - | 4 | - | 11 | - | |
| 2 | Aerobic ATP rephosph (gluc) | ATP-energy(c) | −Glucose +$CO_2$ −$O_2$ =$H_2O$ | Aerobic rephosphorylation of cytosolic ATP from glucose | 0.19 $O_2$(s) 0.03 Glucose(s) | 0.19 $H_2O$(s) 0.19 $CO_2$(s) 1 ATP-energy(c) | 13 | 11 | - | - | - | - | - | - | 4 | - | 11 | - | |
| 3 | Anaerobic rephosph of ATP | ATP-energy(c) | −Glucose +L-Lactate +$CO_2$ =$H_2O$ =Proton-gradient(c) | Anaerobic rephosphorylation of cytosolic ATP from glucose | 0.5 Glucose(s) | 1 L-Lactate(s) 1 ATP-energy(c) 1 Proton-gradient(c) | 12 | - | - | - | - | - | - | - | 3 | - | - | - | |
| 4 | Aerobic rephosph of GTP | GTP(c) | −Palmitate −$P_i$(c) −GDP(c) +$CO_2$ −$O_2$ =$H_2O$ | Aerobic rephosphorylation of cytosolic GTP from glucose | 0.22 $O_2$(s) 1 $P_i$(c) 1 GDP(c) 0.01 Palmitate(s) | 1.15 $H_2O$(s) 0.15 $CO_2$(s) 1 GTP(c) | 5 | 38 | - | - | - | - | - | - | 4 | - | 11 | - | |
| 5 | Aerobic rephosph of CTP | CTP(c) | −Palmitate −$P_i$(c) −UTP(c) −CDP(c) =Glutamine =Glutamate +$CO_2$ −$O_2$ =$H_2O$ | Aerobic rephosphorylation of cytosolic CTP from glucose | 0.15 $O_2$(s) 0.8 $P_i$(c) 0.1 UTP(c) 0.95 CDP(c) | 0.85 $H_2O$(s) 0.2 $CO_2$(s) 0.05 Glutamate(s) 1 CTP(c) | 29 | 13 | - | - | - | - | - | - | 4 | - | 15 | - | |
| 6 | Aerobic rephosph of UDP | UDP(c) | −Palmitate −$P_i$(c) −UMP(c) +$CO_2$ −$O_2$ =$H_2O$ | Aerobic rephosphorylation of cytosolic UDP from glucose | 0.22 $O_2$(s) 1 $P_i$(c) 1 UMP(c) 0.01 Palmitate(s) | 1.15 $H_2O$(s) 0.15 $CO_2$(s) 1 UDP(c) | 6 | 38 | - | - | - | - | - | - | 4 | - | 11 | - | |

Continued on next page

A1. pure energy – continued.

| Simulation | | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 7 | Aerobic rephosph of UTP | UTP(c) | −Palmitate −$P_i$(c) −UDP(c) +$CO_2$ −$O_2$ =$H_2O$ | Aerobic rephospho-rylation of cytosolic UTP from glucose | 0.22 $O_2$(s) 1 $P_i$(c) 1 UDP(c) 0.01 Palmitate(s) | 1.15 $H_2O$(s) 0.15 $CO_2$(s) 1 UTP(c) | 6 | 38 | - | - | - | - | - | - | 4 | - | 11 | - |
| 8 | Anaerobic rephosph of GTP | GTP(c) | −Glucose −$P_i$(c) −GDP(c) +L-Lactate +$CO_2$ =$H_2O$ =Proton-gradient(c) | Anaerobic rephospho-rylation of cytosolic GTP from glucose | 1 $P_i$(c) 0.5 Glucose(s) 1 GDP(c) | 1 $H_2O$(s) 1 GTP(c) 1 L-Lactate(s) 1 Proton-gradient(c) | 12 | - | - | - | - | - | - | - | 4 | - | - | - |
| 9 | Anaerobic rephosph of CTP | CTP(c) | −Glucose −$P_i$(c) −CDP(c) +L-Lactate +$CO_2$ =$H_2O$ =Proton-gradient(c) | Anaerobic rephospho-rylation of cytosolic CTP from glucose | 1 $P_i$(c) 0.5 Glucose(s) 1 CDP(c) | 1 $H_2O$(s) 1 CTP(c) 1 L-Lactate(s) 1 Proton-gradient(c) | 12 | - | - | - | - | - | - | - | 4 | - | - | - |
| 10 | Anaerobic rephosph of UTP | UTP(c) | −Glucose −$P_i$(c) −UDP(c) +L-Lactate +$CO_2$ =$H_2O$ =Proton-gradient(c) | Anaerobic rephospho-rylation of cytosolic UTP from glucose | 1 $P_i$(c) 1 UDP(c) 0.5 Glucose(s) | 1 $H_2O$(s) 1 UTP(c) 1 L-Lactate(s) 1 Proton-gradient(c) | 12 | - | - | - | - | - | - | - | 4 | - | - | - |
| 11 | ATP from NADH(m) | ATP-energy(m) | =NADH-redox-potential(m) =$H_2O$ −$O_2$ %r0205 %r0820 %r0083 | test that $NADH/NAD^+$ potential can be transformed to ATP/ADP potential | 0.15 $O_2$(s) 0.3 NADH-redox-potential(m) | 0.3 $H_2O$(s) 1 ATP-energy(m) | - | 2 | - | - | - | - | - | - | 2 | - | 6 | - |
| 12 | ATP from NADH | ATP-energy(c) | =NADH-redox-potential(c) =$H_2O$ −$O_2$ | test that $NADH/NAD^+$ potential can be transformed to ATP/ADP potential | 0.33 $O_2$(s) 0.67 NADH-redox-potential(c) | 0.67 $H_2O$(s) 1 ATP-energy(c) | 3 | - | - | - | - | - | - | - | 2 | - | 8 | - |

Continued on next page

A1. pure energy – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 13 NADH potential transport | NADH-redox-potential(m) | =NADH-redox-potential(c) $=H_2O$ $-O_2$ | $NADH/NAD^+$ potential transport from the cytosol into the mitochondrium | 0.08 $O_2$(s) 1.17 NADH-redox-potential(c) | 0.17 $H_2O$(s) 1 NADH-redox-potential(m) | 4 | 3 | - | - | - | - | - | - | 2 | - | 7 | - | |
| 14 Ubiquinol-to-ATP | ATP(c) | $-$ADP(c) $-P_i$(c) +Ubiquinone(m) $-$Ubiquinol(m) $=H_2O$(m) $-O_2$(m) | test that mitochondrial ATP/ADP potential without any exchange of substrates | 0.33 $O_2$(m) 1 ADP(c) 1 $P_i$(c) 0.67 Ubiquinol(m) | 1.67 $H_2O$(m) 1 ATP(c) 0.67 Ubiquinone(m) | - | - | - | - | - | - | - | - | - | - | 5 | - | |
| 15 Dephosphorylation of ATP | -1 ATP-energy(c) | $-$Palmitate $+CO_2$ $-O_2$ $=H_2O$ | Dephosphorylation of ATP, release of energy | 1 ATP-energy(c) | | 3 | - | - | - | - | - | - | - | - | - | - | - | |
| **A1.2. NAD(P)H, FADH** | | | | | | | | | | | | | | | | | | |
| 16 Aerobic reduction of $NAD^+$ (FA) | NADH-redox-potential(c) | $-$Palmitate $+CO_2$ $-O_2$ $=H_2O$ | Aerobic reduction of $NAD^+$ | 0.48 $H_2O$(s) 0.24 $O_2$(s) 0.03 Palmitate(s) | 0.52 $CO_2$(s) 1 NADH-redox-potential(c) | 16 | 38 | - | - | - | - | - | - | 4 | - | 14 | - | |
| 17 Aerobic reduction of $NAD^+$ (gluc) | NADH-redox-potential(c) | $-$Glucose $+CO_2$ $-O_2$ $=H_2O$ | Aerobic reduction of $NAD^+$ | 0.49 $H_2O$(s) 0.01 $O_2$(s) 0.09 Glucose(s) | 0.51 $CO_2$(s) 1 NADH-redox-potential(c) | 27 | 8 | - | - | - | - | - | - | 4 | - | 13 | - | |
| 18 Aerobic reduction of $NADP^+$ (FA) | NADPH-redox-potential(c) | $-$Palmitate $+CO_2$ $-O_2$ $=H_2O$ | Aerobic reduction of $NADP^+$ | 0.48 $H_2O$(s) 0.24 $O_2$(s) 0.03 Palmitate(s) | 0.52 $CO_2$(s) 1 NADPH-redox-potential(c) | 12 | 38 | - | - | - | - | - | - | 4 | - | 14 | - | |
| 19 Aerobic reduction of $NADP^+$ (gluc) | NADPH-redox-potential(c) | $-$Glucose $+CO_2$ $-O_2$ $=H_2O$ | Aerobic reduction of $NADP^+$ | 0.49 $H_2O$(s) 0.01 $O_2$(s) 0.09 Glucose(s) | 0.51 $CO_2$(s) 1 NADPH-redox-potential(c) | 24 | 10 | - | - | - | - | - | - | 4 | - | 12 | - | |
| 20 Aerobic reduction of FAD (gluc) | FADH-redox-potential(c) | $-$Glucose $+CO_2$ $-O_2$ $=H_2O$ | Aerobic reduction of FAD | 0.88 $O_2$(s) 0.1 Glucose(s) | 0.13 $H_2O$(s) 1.13 $CO_2$(s) 1 FADH-redox-potential(c) | 65 | 50 | - | - | - | - | - | - | 4 | - | 19 | - | |
| 21 Aerobic reduction of FAD (FA) | FADH-redox-potential(c) | $-$Palmitate $+CO_2$ $-O_2$ $=H_2O$ | Aerobic reduction of FAD | 1.04 $O_2$(s) 0.03 Palmitate(s) | 0.05 $H_2O$(s) 1.05 $CO_2$(s) 1 FADH-redox-potential(c) | 56 | 50 | - | - | - | - | - | - | 4 | - | 19 | - | |

Continued on next page

A1. pure energy – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 22 Oxidation of NADH | -1 NADH-redox-potential(c) | −Palmitate +$CO_2$ −$O_2$ =$H_2O$ %r1414 %r0201 | Oxydation of NADH, release of energy | 0.5 $O_2$(s) 1 NADH-redox-potential(c) | 1 $H_2O$(s) | 3 | 6 | - | - | - | - | - | - | 2 | - | 8 | - |
| 23 Oxidation of NADPH | -1 NADPH-redox-potential(c) | −Palmitate +$CO_2$ −$O_2$ =$H_2O$ %r1414 %r0201 | Oxydation of NADPH, release of energy | 0.5 $O_2$(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) | 3 | 6 | - | - | - | - | - | - | 2 | - | 8 | - |
| 24 NADH redox potential into mito | NADH-redox-potential(m) | −NADH-redox-potential(c) %r0750 | transport of redox potential | 1 NADH-redox-potential(c) | 1 NADH-redox-potential(m) | 5 | 3 | - | - | - | - | - | - | - | - | 2 | - |
| 25 NADH redox potential into peroxy | NADH-redox-potential(p) | −NADH-redox-potential(c) | transport of redox potential | 1 NADH-redox-potential(c) | 1 NADH-redox-potential(p) | 2 | - | - | 2 | - | - | - | - | - | - | 2 | - |
| 26 NADPH redox potential into mito | NADPH-redox-potential(m) | −NADPH-redox-potential(c) | transport of redox potential | 1 NADPH-redox-potential(c) | 1 NADPH-redox-potential(m) | 3 | 3 | - | - | - | - | - | - | - | - | 2 | - |
| 27 NADPH redox potential into peroxy | NADPH-redox-potential(p) | −NADPH-redox-potential(c) | transport of redox potential | 1 NADPH-redox-potential(c) | 1 NADPH-redox-potential(p) | 3 | - | - | 3 | - | - | - | - | - | - | 2 | - |
| 28 NADPH to NADH transhydrogenase | NADH-redox-potential(c) | −NADPH-redox-potential(c) %r0427 %r0750 %r0746 %r0236 | | 1 NADPH-redox-potential(c) | 1 NADH-redox-potential(c) | 4 | - | - | - | - | - | - | - | - | - | - | - |
| 29 NADH to NADPH transhydrogenase | NADPH-redox-potential(c) | −NADH-redox-potential(c) %r0427 %r0750 %r0746 %r0236 | | 1 NADH-redox-potential(c) | 1 NADPH-redox-potential(c) | 4 | - | - | - | - | - | - | - | - | - | - | - |
| 30 NADPH to NADH transhydrogenase in mito | NADH-redox-potential(m) | −NADPH-redox-potential(m) %r0525 | | 1 NADPH-redox-potential(m) | 1 NADH-redox-potential(m) | - | 4 | - | - | - | - | - | - | - | - | - | - |
| 31 NADH to NADPH transhydrogenase in mito | NADPH-redox-potential(m) | −NADH-redox-potential(m) %r0525 | | 1 NADH-redox-potential(m) | 1 NADPH-redox-potential(m) | - | 4 | - | - | - | - | - | - | - | - | - | - |
| **A1.3. Other redox equivalents** | | | | | | | | | | | | | | | | | |

Continued on next page

A1. pure energy – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 32 Thioredoxin(m) reduction | Thioredoxin-redox-potential(m) | −NADPH-redox-potential(m) | test that cytosolic thioredoxin can be reduced using the minimal exchange set | 1 NADPH-redox-potential(m) | 1 Thioredoxin-redox-potential(m) | - | 3 | - | - | - | - | - | - | - | - | - | - |
| 33 Thioredoxin(m) oxidation | -1 Thioredoxin-redox-potential(m) | =NADPH-redox-potential(m) −Palmitate +$CO_2$ −$O_2$ =$H_2O$ | test that cytosolic thioredoxin can be reduced using the minimal exchange set | 1 Thioredoxin-redox-potential(m) | 1 NADPH-redox-potential(m) | - | 3 | - | - | - | - | - | - | - | - | - | - |
| 34 Thioredoxin(c) reduction | Thioredoxin-redox-potential(c) | =NADH-redox-potential(c) −Palmitate +$CO_2$ −$O_2$ =$H_2O$ | test that cytosolic thioredoxin can be reduced using the minimal exchange set | 1 NADH-redox-potential(c) | 1 Thioredoxin-redox-potential(c) | 5 | - | - | - | - | - | - | - | - | - | - | - |
| 35 Thioredoxin(c) oxidation | -1 Thioredoxin-redox-potential(c) | =NADH-redox-potential(c) −Palmitate +$CO_2$ −$O_2$ =$H_2O$ | test that cytosolic thioredoxin can be reduced using the minimal exchange set | 1 Thioredoxin-redox-potential(c) | 1 NADH-redox-potential(c) | 5 | - | - | - | - | - | - | - | - | - | - | - |
| 36 GSH reduction using NADH redox potential | GSH-potential(c) | =NADH-redox-potential(c) | Regeneration of Gluthatione redox potential | 0.5 NADH-redox-potential(c) | 1 GSH-potential(c) | 5 | - | - | - | - | - | - | - | - | - | - | - |
| 37 GSH reduction using NADPH redox potential | GSH-potential(c) | =NADPH-redox-potential(c) | Regeneration of Gluthatione redox potential | 0.5 NADPH-redox-potential(c) | 1 GSH-potential(c) | 3 | - | - | - | - | - | - | - | - | - | - | - |
| 38 GSH oxidation | -1 GSH-potential(c) | =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) | Oxidation of Gluthatione | 1 GSH-potential(c) | 0.5 NADPH-redox-potential(c) | 3 | - | - | - | - | - | - | - | - | - | - | - |

## 2.2 A2. Membrane gradients

Table 2: A2. Membrane gradients

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | | |
| **A2.1. Mitochondrial protons** | | | | | | | | | | | | | | | | | | | |
| 39 Proton-gradient(m) build up | Proton-gradient(m) | $-$Palmitate $+CO_2$ $-O_2$ $=H_2O$ | mitochondrial Proton-gradient build up, protons pumped from the mitochondrial matrix into the cytosol | 0.06 $O_2$(s) 0.003 Palmitate(s) | 0.04 $H_2O$(s) 0.04 $CO_2$(s) 1 Proton-gradient(m) | 4 | 41 | - | - | - | - | - | - | 4 | - | 10 | - | | |
| **A2.2. Plasma membrane protons** | | | | | | | | | | | | | | | | | | | |
| 40 Proton-gradient(c) build up | Proton-gradient(m) | $-$Palmitate $+CO_2$ $-O_2$ $=H_2O$ | apical membrane Proton-gradient build up, protons pumped from the sinusouid into the cytosol | 0.06 $O_2$(s) 0.003 Palmitate(s) | 0.04 $H_2O$(s) 0.04 $CO_2$(s) 1 Proton-gradient(m) | 4 | 41 | - | - | - | - | - | - | 4 | - | 10 | - | | |
| **A2.3. Sodium gradients** | | | | | | | | | | | | | | | | | | | |
| 41 Na+ importgradient | Na+(s) | $-$Na+(c) $-$Palmitate $-O_2$ $+CO_2$ $+H_2O$ | tests that natrium can be pumped out the cell | 0.22 $O_2$(s) 0.01 Palmitate(s) 1 Na+(c) | 0.15 $H_2O$(s) 0.15 $CO_2$(s) 1 Na+(s) | 5 | 38 | - | - | - | - | - | - | 8 | - | 11 | - | | |
| 42 Na+ exportgradient | Na+(c) | $-$Na+(s) $-$Palmitate $-O_2$ $+CO_2$ $+H_2O$ | tests that natrium can be pumped into of the cell | 1 Na+(s) | 1 Na+(c) | - | - | - | - | - | - | - | - | 2 | - | - | - | | |

## 2.3 A3. Small groups activated

Table 3: A3. Small groups activated

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| **A3.1. Methyl(ene) group** | | | | | | | | | | | | | | | | | |
| 43 Activated methyl group (SAM) | Activated methyl group(c) | −Serine +Glycine −ATP-energy(c) =NADPH-redox-potential(c) =$H_2O$ | de novo synthesis of cytosolic Activated methyl group | 1 Serine(s) 3 ATP-energy(c) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 Glycine(s) 1 Activated methyl group(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 44 Activated methyl group (THF) | THF-activated methyl group(c) | −Serine +Glycine −ATP-energy(c) =NADPH-redox-potential(c) =$H_2O$ | de novo synthesis of cytosolic Activated methyl group | 1 Serine(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 Glycine(s) 1 THF-activated methyl group(c) | 4 | - | - | - | - | - | - | - | 2 | - | - | - |
| 45 Activated methylene group from Try | THF-activated methylene group(m) | −Tryptophan +Urea −Palmitate +$CO_2$ −$O_2$ =$H_2O$ | de novo synthesis of mitochondrial Activated methyl group | 10.5 $O_2$(s) 1 Tryptophan(s) | 4 $H_2O$(s) 9 $CO_2$(s) 1 Urea(s) 1 THF-activated methylene group(m) | 30 | 23 | - | - | - | - | - | - | 5 | - | 18 | - |
| 46 Activated methyl group from Histidine | THF-activated methyl group(c) | −Histidine +Urea −ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =$H_2O$ −$O_2$ +$CO_2$ −$NH_3$ %r1414 | de novo synthesis of cytosolic Activated methyl group | 5.34 $H_2O$(s) 0.58 $O_2$(s) 1 Histidine(s) 4.92 ATP-energy(c) | 3.5 $CO_2$(s) 1.5 Urea(s) 0.5 NADH-redox-potential(c) 5.34 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 41 | 12 | - | - | - | - | - | - | 6 | - | 15 | - |
| **A3.2. Formyl group** | | | | | | | | | | | | | | | | | |
| 47 Formylgroup(c) | THF-activated formyl group(c) | −Serine +Glycine −ATP-energy(c) =NADPH-redox-potential(c) =$H_2O$ | test that the methyl group on THF can be regenerated from the minimal exchange set | 1 Serine(s) | 1 Glycine(s) 1 NADPH-redox-potential(c) 1 THF-activated formyl group(c) | 5 | - | - | - | - | - | - | - | 1 | - | - | - |

Continued on next page

A3. Small groups activated – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 48 Formylgroup(m) | THF-activated formyl group(m) | −Serine +Glycine −ATP-energy(c) =NADPH-redox-potential(c) =$H_2O$ +Urea −Palmitate −$O_2$ +$CO_2$ +Glutamine(c) +Glutamate(c) −Tryptophan(c) | test that the methyl group on THF can be regenerated from the minimal exchange set | 1.8 $H_2O$(s) 3.6 $O_2$(s) 1 Serine(s) 1 Tryptophan(c) 1 ATP-energy(c) | 3 $CO_2$(s) 1 Glutamate(c) 1 Glutamine(c) 1.8 NADPH-redox-potential(c) 1 THF-activated formyl group(m) | 17 | 16 | - | - | - | - | - | - | 4 | - | 15 | - |
| **A3.3. Acetyl group** | | | | | | | | | | | | | | | | | |
| 49 Acetyl group(c) | CoA-activated acetyl group(c) | −Palmitate −$O_2$ =$H_2O$ =Proton-gradient(m) +ATP-energy(m) =ATP-energy(c) =NADH-redox-potential(m) | Regeneration of Acetyl-CoA minus CoA | 0.44 $O_2$(s) 0.13 Palmitate(s) 2.25 ATP-energy(c) | 0.13 $H_2O$(s) 0.88 NADH-redox-potential(m) 5.25 Proton-gradient(m) 1 CoA-activated acetyl group(c) | 7 | 31 | - | - | - | - | - | - | 3 | - | 7 | - |
| 50 Acetyl group(m) | CoA-activated acetyl group(m) | −Palmitate −$O_2$ =$H_2O$ =Proton-gradient(m) +ATP-energy(m) =ATP-energy(c) =NADH-redox-potential(m) | Regeneration of Acetyl-CoA minus CoA | 0.44 $O_2$(s) 0.13 Palmitate(s) 0.25 ATP-energy(c) | 0.13 $H_2O$(s) 0.88 NADH-redox-potential(m) 5.25 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 5 | 31 | - | - | - | - | - | - | 3 | - | 5 | - |
| 51 Acetyl group(p) | CoA-activated acetyl group(p) | −Palmitate −$O_2$ =$H_2O$ =Proton-gradient(m) +ATP-energy(m) =ATP-energy(c) =NADH-redox-potential(m) | Regeneration of Acetyl-CoA minus CoA | 0.44 $O_2$(s) 0.13 Palmitate(s) 2.25 ATP-energy(c) | 0.13 $H_2O$(s) 0.88 NADH-redox-potential(m) 5.25 Proton-gradient(m) 1 CoA-activated acetyl group(p) | 7 | 31 | - | 2 | - | - | - | - | 3 | - | 8 | - |
| 52 Acetyl group(r) | CoA-activated acetyl group(r) | −Palmitate −$O_2$ =$H_2O$ =Proton-gradient(m) +ATP-energy(m) =ATP-energy(c) =NADH-redox-potential(m) | Regeneration of Acetyl-CoA minus CoA | 0.44 $O_2$(s) 0.13 Palmitate(s) 2.25 ATP-energy(c) | 0.13 $H_2O$(s) 0.88 NADH-redox-potential(m) 5.25 Proton-gradient(m) 1 CoA-activated acetyl group(r) | 6 | 31 | 1 | - | - | - | - | - | 3 | - | 9 | - |
| **A3.4. Sulfate group** | | | | | | | | | | | | | | | | | |

Continued on next page

A3. Small groups activated – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 53 activated sulphur | activated-sulphur(c) | −Sulfate(c) =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) $-O_2$ $+CO_2$ $=H_2O$ | Regeneration of cytosolic activated-sulphur | 1 Sulfate(c) 3 ATP-energy(c) | 1 $H_2O$(s) 1 activated-sulphur(c) | 7 | - | - | - | - | - | - | - | 1 | - | - | - |

## 2.4 A4. Activated sugars

Table 4: A4. Activated sugars

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| **A4.1. Glucose-6-P** | | | | | | | | | | | | | | | | | |
| 54 Glucose-6P | Glucose-6P(c) | −Glucose =ATP-energy(c) =$P_i$(c) =$H_2O$ | Synthesis of Glucose-6P | 1 $P_i$(c) 1 Glucose(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Glucose-6P(c) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |
| **A4.2. UDP-activated sugars** | | | | | | | | | | | | | | | | | |
| 55 UDP-activated glucose | UDP-activated-glucose(c) | −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) $-O_2$ $+CO_2$ $+H_2O$ =$P_i$(c) | Regeneration of UDP glucose minus UDP | 1 Glucose-6P(c) 1 ATP-energy(c) | 1 $P_i$(c) 1 UDP-activated-glucose(c) | 6 | - | - | - | - | - | - | - | - | - | - | - |
| 56 UDP-activated glucuronate | UDP-activated-glucuronate(c) | −Glucose-6P(c) =ATP-energy(c) =Proton-gradient(m) $-O_2$ $+CO_2$ $+H_2O$ =$P_i$(c) %r1239 %r1414 | Regeneration of UDP glucuronate minus UDP | 1 $O_2$(s) 1 Glucose-6P(c) 1 ATP-energy(c) | 1 $H_2O$(s) 1 $P_i$(c) 12 Proton-gradient(m) 1 UDP-activated-glucuronate(c) | 8 | - | - | - | - | - | - | - | 2 | - | 6 | - |
| 57 UDP-activated galactose | UDP-activated-galactose(c) | −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =$H_2O$ =$P_i$(c) =NADPH-redox-potential(c) | Regeneration of UDP-activated galactose | 1 Glucose-6P(c) 1 ATP-energy(c) | 1 $P_i$(c) 1 UDP-activated-galactose(c) | 7 | - | - | - | - | - | - | - | - | - | - | - |

Continued on next page

A4. Activated sugars – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| **A4.3. Other nucleosides-activated sugars** | | | | | | | | | | | | | | | | | |
| 58 GDP-activated fucose | GDP-activated-fucose(c) | −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =$H_2O$ =$P_i$(c) =NADPH-redox-potential(c) | Regeneration of GDP-activated fucose | 1 Glucose-6P(c) 1 ATP-energy(c) 1 NADH-redox-potential(c) | 1 $H_2O$(s) 1 $P_i$(c) 1 GDP-activated-fucose(c) | 11 | - | - | - | - | - | - | - | 1 | - | - | - |
| 59 GDP-activated mannose | GDP-activated-mannose(c) | −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =$H_2O$ =$P_i$(c) =NADPH-redox-potential(c) | Regeneration of GDP-activated mannose | 1 Glucose-6P(c) 1 ATP-energy(c) | 1 $P_i$(c) 1 GDP-activated-mannose(c) | 8 | - | - | - | - | - | - | - | - | - | - | - |

## 2.5 A5. Important intermediates



Table 5: A5. Important intermediates

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| **A5.1. Pyruvate** | | | | | | | | | | | | | | | | | |
| 60 Pyruvate | Pyruvate(c) | −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =$H_2O$ =$P_i$(c) =NADPH-redox-potential(c) | Synthesis of Pyruvate | 0.5 $H_2O$(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 1 Pyruvate(c) 1.5 ATP-energy(c) 1 NADH-redox-potential(c) | 11 | - | - | - | - | - | - | - | 1 | - | - | - |
| **A5.2. AKG** | | | | | | | | | | | | | | | | | |

Continued on next page

A5. Important intermediates – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 61 AKG | AKG(c) | −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =NADH-redox-potential(m) =$H_2O$ =$P_i$(c) =NADPH-redox-potential(m) =NADPH-redox-potential(c) =$CO_2$(m) =$CO_2$(c) =CoA-activated acetyl group(m) | Synthesis of AKG | 1.5 $H_2O$(s) 1 $CO_2$(c) 0.5 Glucose-6P(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(m) | 0.5 $P_i$(c) 1 $CO_2$(m) 1 AKG(c) 1.5 ATP-energy(c) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(m) | 13 | 8 | - | - | - | - | - | - | 1 | - | 2 | - |
| **A5.3. Terpenoids** | | | | | | | | | | | | | | | | | |
| 62 Isopentenyl-PP | Isopentenyl-PP(p) | −Acetyl-CoA(c) +CoA(c) =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =$H_2O$ =$P_i$(c) =$CO_2$ | synthesis of peroxysomal Isopentenyl-PP | 2 $P_i$(c) 3 Acetyl-CoA(c) 3 ATP-energy(c) 2 NADPH-redox-potential(c) | 2 $H_2O$(s) 3 CoA(c) 1 $CO_2$(s) 1 Isopentenyl-PP(p) | 5 | - | - | 3 | - | - | - | - | 2 | - | 4 | - |
| 63 Farnesyl-PP | Farnesyl-PP(p) | −Acetyl-CoA(c) +CoA(c) =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =$H_2O$ =$P_i$(c) =$CO_2$ | de novo synthesis of peroxysomal Farnesyl-PP | 2 $P_i$(c) 9 Acetyl-CoA(c) 9 ATP-energy(c) 6 NADPH-redox-potential(c) | 4 $H_2O$(s) 9 CoA(c) 3 $CO_2$(s) 1 Farnesyl-PP(p) | 6 | - | - | 6 | - | - | - | - | 2 | - | 5 | - |
| **A5.4. Aminosugars** | | | | | | | | | | | | | | | | | |

Continued on next page

A5. Important intermediates – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 64 Glucosamine-6P | Glucosamine-6P(c) | −CoA-activated acetyl group(c) +Glutamate =Na-gradient(c) −Glutamine −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =$H_2O$ =$P_i$(c) =$CO_2$ | synthesis of D-Glucosamine 6-phosphate from activated acetyl and Glutamine minus Glutamate | 1 Glutamine(s) 1 Glucose-6P(c) | 1 Glutamate(s) 1 Glucosamine-6P(c) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |

## 2.6 A6. Salvage

Table 6: A6. Salvage

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 65 ATP salvage from Adenosine | ATP(c) | −Adenosine(c) =ATP-energy(c) =NADH-redox-potential(c) −$P_i$(c) +$CO_2$ −$O_2$ =$H_2O$ | ATP salvage from Adenosine | 3 $P_i$(c) 1 Adenosine(c) 3 ATP-energy(c) | 3 $H_2O$(s) 1 ATP(c) | 3 | - | - | - | - | - | - | - | 1 | - | - | - |
| 66 ATP salvage from Hypoxanthine | ATP(c) | −Hypoxanthine(c) −Glucose-6P(c) −Pyruvate(c) =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =NADH-redox-potential(m) =NADPH-redox-potential(m) −$P_i$(c) −Glutamine(c) +$CO_2$ −$O_2$ =$H_2O$ | ATP salvage from Hypoxanthine | 0.25 $O_2$(s) 2.42 $P_i$(c) 0.5 Glutamine(c) 0.58 Glucose-6P(c) 1 Hypoxanthine(c) 5.42 ATP-energy(c) | 2.92 $H_2O$(s) 1 ATP(c) 1 $CO_2$(s) 0.5 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) | 26 | 9 | - | - | - | - | - | - | 3 | - | 11 | - |

Continued on next page

A6. Salvage – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 67 dTTP salvage from Thymine | dTTP(c) | −Thymine(c) −Glucose-6P(c) =ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =NADH-redox-potential(m) =NADPH-redox-potential(m) $-P_i$(c) $+CO_2$ $-O_2$ $=H_2O$ | dTTP salvage from Thymine | 2.17 $P_i$(c) 0.83 Glucose-6P(c) 1 Thymine(c) 5.17 ATP-energy(c) 1 NADPH-redox-potential(c) | 4.17 $H_2O$(s) 1 dTTP(c) | 24 | - | - | - | - | - | - | - | 1 | - | - | - |

## 2.7 A7. Detoxification of internally emerging substances

Table 7: A7. Detoxification of internally emerging substances

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 68 $O_2$.-(c) degr | -1 $O_2$.-(c) | MCES $=O_2$ | degradation of cytosolic $O_2$.- | 1 $O_2$.-(c) | 0.5 $H_2O$(s) 0.75 $O_2$(s) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |
| 69 Formaldehyde degr | -1 Formaldehyde | MCES | degradation of external formaldehyde | 1 Formaldehyde(s) 1 ATP-energy(c) | 0.5 $CO_2$(s) 0.5 NADH-redox-potential(c) 0.5 THF-activated methyl group(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 70 Formate degr | -1 Formate | MCES | degradation of external formate | 1 Formate(s) 1 ATP-energy(c) 1 Proton-gradient(c) | 1 $CO_2$(s) 1 NADPH-redox-potential(c) | 4 | - | - | - | - | - | - | - | 4 | - | - | - |

# 3 B. Functions of organismic duty

## 3.1 B1. Storage/Release

Table 8: B1. Storage/Release

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| **B1.1. Glycogen** | | | | | | | | | | | | | | | | | | |
| 71 Glycogen glucose storage | Glycogenin-G4G7(c) | −Glycogenin(c) −UDP-activated-glucose(c) | test the storage of glucose in a glycogen component | 1 Glycogenin(c) 11 UDP-activated-glucose(c) | 1 Glycogenin-G4G7(c) | 4 | - | - | - | - | - | - | - | - | - | - | - | - |
| 72 Glycogen glucose release | Glucose | −Glycogenin-G4G7(c) +Glycogenin(c) −Glucose $-O_2$ $+CO_2$ $=H_2O$ | test the release of glucose from a glycogen component | 1 $H_2O$(s) 0.09 Glycogenin-G4G7(c) | 1 Glucose(s) 0.09 Glycogenin(c) | 5 | - | 1 | - | - | - | - | - | 2 | - | 3 | - | - |

## 3.2 B2. Turnover functions

Table 9: B2. Turnover functions

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| **B2.1. Gluconeogenesis** | | | | | | | | | | | | | | | | | | |
| 73 Gluconeogen from Lactate | Glucose | −L-Lactate(c) −ATP-energy(m) −ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =NADH-redox-potential(m) =NADPH-redox-potential(m) =Proton-gradient(m) $=H_2O$ $=CO_2$ $=O_2$ | Gluconeogenese from Lactate | 2 L-Lactate(c) 2 ATP-energy(c) 2 ATP-energy(m) 2 NADPH-redox-potential(m) 2 Proton-gradient(m) | 1 Glucose(s) 2 NADH-redox-potential(m) | 10 | 7 | 1 | - | - | - | - | - | 1 | - | 9 | - | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 74 | Gluconeogen from Glycerol | Glucose | −Glycerol −ATP-energy(m) −ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =Proton-gradient(m) =$H_2O$ =$CO_2$ =$O_2$ %r0530 | Gluconeogenese from Glycerol | 1 $O_2$(s) 2 Glycerol(s) 2 ATP-energy(c) | 2 $H_2O$(s) 1 Glucose(s) 12 Proton-gradient(m) | 6 | - | 1 | - | - | - | - | - | 4 | - | 9 | - |
| 75 | Gluconeogen from Alanine | Glucose | −Alanine −ATP-energy(m) −ATP-energy(c) =NADH-redox-potential(c) =NADPH-redox-potential(c) =Proton-gradient(m) =$H_2O$ =$CO_2$ =$O_2$ +Urea | Gluconeogenese from Alanine | 1 $H_2O$(s) 1 $CO_2$(s) 2 Alanine(s) 5 ATP-energy(c) 3 ATP-energy(m) 1 NADPH-redox-potential(c) | 1 Glucose(s) 1 Urea(s) 1 NADH-redox-potential(c) | 23 | 7 | 1 | - | - | - | - | - | 5 | - | 9 | - |
| | **B2.2. Amino acid nxn** | | | | | | | | | | | | | | | | | |
| 76 | Alanine from Arginine | Alanine | −Arginine MCES +Urea | Transamination to Alanine using Arginine | 1.5 $H_2O$(s) 0.25 $O_2$(s) 0.5 Pyruvate(m) 0.5 Arginine(s) 0.5 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Alanine(s) 0.5 Urea(s) 0.5 ATP-energy(m) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1.5 Proton-gradient(m) | 4 | 11 | - | - | - | - | - | - | 7 | - | 10 | - |
| 77 | Alanine from Asparagine | Alanine | −Asparagine MCES +Urea | Transamination to Alanine using Asparagine | 0.5 Pyruvate(c) 0.5 Asparagine(s) 0.5 NADH-redox-potential(c) 0.5 NADPH-redox-potential(m) 1 Proton-gradient(m) | 0.5 $CO_2$(s) 1 Alanine(s) 0.5 NADPH-redox-potential(c) | 7 | 2 | - | - | - | - | - | - | 4 | - | 7 | - |
| 78 | Alanine from Aspartate | Alanine | −Aspartate MCES +Urea | Transamination to Alanine using Aspartate | 1 Aspartate(s) 1 NADH-redox-potential(c) | 1 $CO_2$(s) 1 Alanine(s) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 6 | - | - | - | - | - | - | - | 4 | - | - | - |
| 79 | Alanine from Cysteine | Alanine | −Cysteine MCES +Urea +$H_2S$ | Transamination to Alanine using Cysteine | 1 Cysteine(s) 1 NADH-redox-potential(m) 2 Proton-gradient(m) | 1 Alanine(s) 1 $H_2S$(s) 1 Na-gradient(c) | 2 | 2 | - | - | - | - | - | - | 4 | - | 7 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 80 Alanine from Cystine | Alanine | −Cystine MCES +Urea +$H_2S$ | Transamination to Alanine using Cystine | 0.5 Cystine(s) 1 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 2 Proton-gradient(m) | 1 Alanine(s) 1 $H_2S$(s) 0.5 Na-gradient(c) | 4 | 2 | - | - | - | - | - | - | 5 | - | 7 | - |
| 81 Alanine from Glutamate | Alanine | −Glutamate MCES +Urea | Transamination to Alanine using Glutamate | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamate(s) | 2 $CO_2$(s) 1 Alanine(s) 1 ATP-energy(m) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 6 Proton-gradient(m) 1 Na-gradient(c) | 3 | 7 | - | - | - | - | - | - | 6 | - | 7 | - |
| 82 Alanine from Glycine | Alanine | −Glycine MCES +Urea | Transamination to Alanine using Glycine | 1 Glycine(s) 1 THF-activated methyl group(c) | 1 Alanine(s) | 9 | - | - | - | - | - | - | - | 1 | - | - | - |
| 83 Alanine from Histidine | Alanine | −Histidine MCES +Urea | Transamination to Alanine using Histidine | 0.33 $H_2O$(s) 0.17 $O_2$(s) 0.33 Pyruvate(c) 0.33 Pyruvate(m) 0.33 Histidine(s) 0.33 NADH-redox-potential(c) 0.33 NADH-redox-potential(m) 0.33 NADPH-redox-potential(m) | 0.67 $CO_2$(s) 1 Alanine(s) 0.33 ATP-energy(m) 0.33 NADPH-redox-potential(c) 1 Proton-gradient(m) 0.33 THF-activated methyl group(c) | 12 | 10 | - | - | - | - | - | - | 6 | - | 11 | - |
| 84 Alanine from Isoleucine | Alanine | −Isoleucine MCES +Urea | Transamination to Alanine using Isoleucine | 1 $H_2O$(s) 1 $O_2$(s) 1 Pyruvate(c) 1 Isoleucine(s) | 2 $CO_2$(s) 1 Alanine(s) 4 NADH-redox-potential(m) 9 Proton-gradient(m) 2 CoA-activated acetyl group(m) | 1 | 13 | - | - | - | - | - | - | 5 | - | 11 | - |
| 85 Alanine from Glutamine | Alanine | −Glutamine MCES +Urea | Transamination to Alanine using Glutamine | 0.5 $H_2O$(s) 0.25 $O_2$(s) 0.5 Pyruvate(c) 0.5 Glutamine(s) 0.5 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Alanine(s) 0.5 ATP-energy(m) 0.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 2 Proton-gradient(m) | 5 | 9 | - | - | - | - | - | - | 5 | - | 11 | - |
| 86 Alanine from Leucine | Alanine | −Leucine MCES +Urea | Transamination to Alanine using Leucine | 0.5 $O_2$(s) 1 Pyruvate(c) 1 Leucine(s) 1 NADPH-redox-potential(m) | 1 $H_2O$(s) 1 Alanine(s) 2 NADH-redox-potential(m) 4 Proton-gradient(m) 1 Na-gradient(c) 3 CoA-activated acetyl group(m) | 1 | 13 | - | - | - | - | - | - | 5 | - | 10 | - |
| 87 Alanine from Lysine | Alanine | −Lysine MCES +Urea | Transamination to Alanine using Lysine | 0.5 $H_2O$(s) 0.25 $O_2$(s) 1 Pyruvate(c) 0.5 Lysine(s) | 1 $CO_2$(s) 1 Alanine(s) 0.5 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 3 | 10 | - | - | - | - | - | - | 5 | - | 11 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 88 | Alanine from Methionine | Alanine | −Methionine MCES +Urea +$H_2S$ | Transamination to Alanine using Methionine | 1.5 $H_2O$(s) 0.5 $O_2$(s) 1 Methionine(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Alanine(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 17 | 9 | - | - | - | - | - | - | 7 | - | 12 | - |
| 89 | Alanine from Phenylalanine | Alanine | −Phenylalanine MCES +Urea | Transamination to Alanine using Phenylalanine | 3 $O_2$(s) 1 Phenylalanine(s) 2 ATP-energy(c) | 2 $CO_2$(s) 1 Alanine(s) 2 CoA-activated acetyl group(c) | 16 | - | - | - | - | - | - | - | 4 | - | - | - |
| 90 | Alanine from Proline | Alanine | −Proline MCES +Urea | Transamination to Alanine using Proline | 4 $H_2O$(s) 1 Proline(s) | 2 $CO_2$(s) 1 Alanine(s) 1 ATP-energy(m) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 3 | 10 | - | - | - | - | - | - | 5 | - | 4 | - |
| 91 | Alanine from Serine | Alanine | −Serine MCES +Urea | Transamination to Alanine using Serine | 1 Serine(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 Alanine(s) | 7 | - | - | - | - | - | - | - | 3 | - | - | - |
| 92 | Alanine from Threonine | Alanine | −Threonine MCES +Urea | Transamination to Alanine using Threonine | 0.5 $O_2$(s) 1 Pyruvate(c) 1 Threonine(s) | 2 $CO_2$(s) 1 Alanine(s) 2 NADH-redox-potential(m) 3 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 2 | 9 | - | - | - | - | - | - | 4 | - | 11 | - |
| 93 | Alanine from Tryptophan | Alanine | −Tryptophan MCES +Urea | Transamination to Alanine using Tryptophan | 1.75 $O_2$(s) 0.5 Pyruvate(c) 0.5 Tryptophan(s) 0.5 ATP-energy(c) 1.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) | 1.5 $CO_2$(s) 1 Alanine(s) 1 NADH-redox-potential(m) 1.5 Proton-gradient(m) 0.5 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 16 | 9 | - | - | - | - | - | - | 5 | - | 12 | - |
| 94 | Alanine from Tyrosine | Alanine | −Tyrosine MCES +Urea | Transamination to Alanine using Tyrosine | 1 $H_2O$(s) 2 $O_2$(s) 1 Tyrosine(s) 2 ATP-energy(c) | 2 $CO_2$(s) 1 Alanine(s) 1 NADPH-redox-potential(c) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 15 | - | - | - | - | - | - | - | 6 | - | - | - |
| 95 | Alanine from Valine | Alanine | −Valine MCES +Urea | Transamination to Alanine using Valine | 2 $H_2O$(s) 1 $O_2$(s) 1 Valine(s) | 2 $CO_2$(s) 1 Alanine(s) 1 ATP-energy(m) 3 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 10 Proton-gradient(m) | 3 | 14 | - | - | - | - | - | - | 5 | - | 10 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 96 Alanine from beta-Alanine | Alanine | −beta-Alanine MCES +Urea | Transamination to Alanine using beta-Alanine | 1 Pyruvate(c) 1 beta-Alanine(s) 2 Proton-gradient(m) | 1 $CO_2$(s) 1 Alanine(s) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 1 | 4 | - | - | - | - | - | - | 3 | - | 7 | - |
| 97 Arginine from Alanine | Arginine | −Alanine MCES +Urea | Transamination to Arginine using Alanine | 4 Alanine(s) 2 ATP-energy(c) 3 ATP-energy(m) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 Pyruvate(c) 1 Pyruvate(m) 1 Arginine(s) 1 NADH-redox-potential(c) 4 NADH-redox-potential(m) 1 Na-gradient(c) | 10 | 17 | - | - | - | - | - | - | 4 | - | 3 | - |
| 98 Arginine from Asparagine | Arginine | −Asparagine MCES +Urea | Transamination to Arginine using Asparagine | 2 Asparagine(s) 3 ATP-energy(c) 3 ATP-energy(m) 1 NADH-redox-potential(c) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Arginine(s) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 13 | 16 | - | - | - | - | - | - | 6 | - | 6 | - |
| 99 Arginine from Aspartate | Arginine | −Aspartate MCES +Urea | Transamination to Arginine using Aspartate | 4 Aspartate(s) 2 ATP-energy(c) 3 ATP-energy(m) 1 NADH-redox-potential(c) 2 Proton-gradient(m) | 5 $CO_2$(s) 1 Pyruvate(c) 1 Arginine(s) 3 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 4 Na-gradient(c) 1 CoA-activated acetyl group(m) | 14 | 14 | - | - | - | - | - | - | 4 | - | 6 | - |
| 100 Arginine from Cysteine | Arginine | −Cysteine MCES +Urea +$H_2S$ | Transamination to Arginine using Cysteine | 2 Pyruvate(m) 4 Cysteine(s) 2 ATP-energy(c) 3 ATP-energy(m) 2 NADPH-redox-potential(m) 3 Proton-gradient(m) | 4 Pyruvate(c) 1 Arginine(s) 4 $H_2S$(s) 1 NADH-redox-potential(c) 4 Na-gradient(c) | 10 | 15 | - | - | - | - | - | - | 5 | - | 8 | - |
| 101 Arginine from Cystine | Arginine | −Cystine MCES +Urea +$H_2S$ | Transamination to Arginine using Cystine | 2 Pyruvate(m) 2 Cystine(s) 2 ATP-energy(c) 3 ATP-energy(m) 2 NADPH-redox-potential(c) 2 NADPH-redox-potential(m) 3 Proton-gradient(m) | 4 Pyruvate(c) 1 Arginine(s) 4 $H_2S$(s) 1 NADH-redox-potential(c) 2 Na-gradient(c) | 12 | 15 | - | - | - | - | - | - | 5 | - | 8 | - |
| 102 Arginine from Glutamate | Arginine | −Glutamate MCES +Urea | Transamination to Arginine using Glutamate | 2 $H_2O$(s) 1.5 $O_2$(s) 4 Glutamate(s) 2 ATP-energy(c) | 5 $CO_2$(s) 1 Pyruvate(c) 2 Pyruvate(m) 1 Arginine(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 3 NADPH-redox-potential(m) 14 Proton-gradient(m) 4 Na-gradient(c) | 11 | 14 | - | - | - | - | - | - | 6 | - | 10 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 103 Arginine from Glycine | Arginine | −Glycine MCES +Urea | Transamination to Arginine using Glycine | 2 Pyruvate(m) 4 Glycine(s) 2 ATP-energy(c) 3 ATP-energy(m) 4 NADPH-redox-potential(m) 1 Proton-gradient(m) 4 THF-activated methyl group(c) | 4 Pyruvate(c) 1 Arginine(s) 1 NADH-redox-potential(c) 3 NADH-redox-potential(m) 3 NADPH-redox-potential(c) 4 Na-gradient(c) | 21 | 16 | - | - | - | - | - | - | 3 | - | 4 | - |
| 104 Arginine from Histidine | Arginine | −Histidine MCES +Urea | Transamination to Arginine using Histidine | 0.17 $O_2$(s) 1.33 Histidine(s) 2 ATP-energy(c) 1.67 ATP-energy(m) 0.67 NADH-redox-potential(m) 0.33 NADPH-redox-potential(c) 1.67 NADPH-redox-potential(m) | 0.33 Pyruvate(c) 1 Arginine(s) 0.33 Na-gradient(c) 1 THF-activated methyl group(c) | 20 | 13 | - | - | - | - | - | - | 5 | - | 11 | - |
| 105 Arginine from Isoleucine | Arginine | −Isoleucine MCES +Urea | Transamination to Arginine using Isoleucine | 2 $H_2O$(s) 3.5 $O_2$(s) 1 Pyruvate(m) 4 Isoleucine(s) 2 ATP-energy(c) 3 ATP-energy(m) 3 NADPH-redox-potential(m) | 4 $CO_2$(s) 1 Pyruvate(c) 1 Arginine(s) 16 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 35 Proton-gradient(m) 1 Na-gradient(c) 7 CoA-activated acetyl group(m) | 8 | 29 | - | - | - | - | - | - | 7 | - | 11 | - |
| 106 Arginine from Glutamine | Arginine | −Glutamine MCES +Urea | Transamination to Arginine using Glutamine | 0.5 $O_2$(s) 2 Glutamine(s) 2 ATP-energy(c) 1 ATP-energy(m) 1 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Arginine(s) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) 4 Proton-gradient(m) 1 Na-gradient(c) | 11 | 13 | - | - | - | - | - | - | 6 | - | 9 | - |
| 107 Arginine from Leucine | Arginine | −Leucine MCES +Urea | Transamination to Arginine using Leucine | 2 $O_2$(s) 2 Pyruvate(m) 4 Leucine(s) 2 ATP-energy(c) 3 ATP-energy(m) 6 NADPH-redox-potential(m) | 4 $H_2O$(s) 1 Arginine(s) 1 NADH-redox-potential(c) 12 NADH-redox-potential(m) 21 Proton-gradient(m) 4 Na-gradient(c) 12 CoA-activated acetyl group(m) | 9 | 25 | - | - | - | - | - | - | 6 | - | 11 | - |
| 108 Arginine from Lysine | Arginine | −Lysine MCES +Urea | Transamination to Arginine using Lysine | 2 $H_2O$(s) 1 $O_2$(s) 2 Pyruvate(m) 2 Lysine(s) 2 ATP-energy(c) 3 ATP-energy(m) 3 NADPH-redox-potential(m) | 3 $CO_2$(s) 1 Pyruvate(c) 1 Arginine(s) 2 NADH-redox-potential(c) 8 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 9 Proton-gradient(m) 3 CoA-activated acetyl group(m) | 10 | 25 | - | - | - | - | - | - | 5 | - | 11 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 109 Arginine from Methionine | Arginine | −Methionine MCES +Urea +$H_2S$ | Transamination to Arginine using Methionine | 4 $H_2O$(s) 1.5 $O_2$(s) 1 Pyruvate(m) 4 Methionine(s) 2 Glucose-6P(c) 3 ATP-energy(m) 3 NADPH-redox-potential(m) | 2 $P_i$(c) 4 $CO_2$(s) 5 Pyruvate(c) 1 Arginine(s) 4 $H_2S$(s) 8 NADH-redox-potential(c) 4 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 3 Proton-gradient(m) 4 Na-gradient(c) 4 THF-activated methyl group(c) 3 CoA-activated acetyl group(m) | 22 | 24 | - | - | - | - | - | - | 8 | - | 14 | - |
| 110 Arginine from Phenylalanine | Arginine | −Phenylalanine MCES +Urea | Transamination to Arginine using Phenylalanine | 12 $O_2$(s) 4 Phenylalanine(s) 10 ATP-energy(c) 3 ATP-energy(m) 2 NADPH-redox-potential(c) 4 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 7 $CO_2$(s) 1 Pyruvate(c) 2 Pyruvate(m) 1 Arginine(s) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 1 Na-gradient(c) 8 CoA-activated acetyl group(c) | 24 | 13 | - | - | - | - | - | - | 6 | - | 6 | - |
| 111 Arginine from Proline | Arginine | −Proline MCES +Urea | Transamination to Arginine using Proline | 13 $H_2O$(s) 4 Proline(s) 2 ATP-energy(c) | 5 $CO_2$(s) 1 Pyruvate(c) 2 Pyruvate(m) 1 Arginine(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 5 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 3 NADPH-redox-potential(m) 1 Na-gradient(c) | 11 | 16 | - | - | - | - | - | - | 6 | - | 8 | - |
| 112 Arginine from Serine | Arginine | −Serine MCES +Urea | Transamination to Arginine using Serine | 2 Pyruvate(m) 4 Serine(s) 2 ATP-energy(c) 3 ATP-energy(m) 1 NADPH-redox-potential(c) 4 NADPH-redox-potential(m) 1 Proton-gradient(m) | 4 $H_2O$(s) 4 Pyruvate(c) 1 Arginine(s) 1 NADH-redox-potential(c) 3 NADH-redox-potential(m) 4 Proton-gradient(c) 4 Na-gradient(c) | 18 | 16 | - | - | - | - | - | - | 5 | - | 4 | - |
| 113 Arginine from Threonine | Arginine | −Threonine MCES +Urea | Transamination to Arginine using Threonine | 1.5 $O_2$(s) 1 Pyruvate(m) 4 Threonine(s) 2 ATP-energy(c) 3 ATP-energy(m) 3 NADPH-redox-potential(m) | 2 $H_2O$(s) 4 $CO_2$(s) 1 Pyruvate(c) 1 Arginine(s) 8 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 11 Proton-gradient(m) 1 Na-gradient(c) 3 CoA-activated acetyl group(m) | 9 | 24 | - | - | - | - | - | - | 7 | - | 12 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 114 Arginine from Tryptophan | Arginine | −Tryptophan MCES +Urea | Transamination to Arginine using Tryptophan | 7 $O_2$(s) 2 Pyruvate(m) 2 Tryptophan(s) 5 ATP-energy(c) 3 ATP-energy(m) 4 NADPH-redox-potential(c) 4 NADPH-redox-potential(m) | 5 $CO_2$(s) 3 Pyruvate(c) 1 Arginine(s) 6 NADH-redox-potential(m) 10 Proton-gradient(m) 1 Na-gradient(c) 2 THF-activated methyl group(c) 3 CoA-activated acetyl group(m) | 26 | 20 | - | - | - | - | - | - | 6 | - | 12 | - |
| 115 Arginine from Tyrosine | Arginine | −Tyrosine MCES +Urea | Transamination to Arginine using Tyrosine | 4 $H_2O$(s) 8 $O_2$(s) 4 Tyrosine(s) 10 ATP-energy(c) 3 ATP-energy(m) 4 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 7 $CO_2$(s) 1 Pyruvate(c) 2 Pyruvate(m) 1 Arginine(s) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 4 Na-gradient(c) 8 CoA-activated acetyl group(c) | 22 | 13 | - | - | - | - | - | - | 6 | - | 6 | - |
| 116 Arginine from Valine | Arginine | −Valine MCES +Urea | Transamination to Arginine using Valine | 6 $H_2O$(s) 3.5 $O_2$(s) 4 Valine(s) 2 ATP-energy(c) | 5 $CO_2$(s) 1 Pyruvate(c) 2 Pyruvate(m) 1 Arginine(s) 1 NADH-redox-potential(c) 12 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 36 Proton-gradient(m) 4 Na-gradient(c) | 11 | 22 | - | - | - | - | - | - | 7 | - | 11 | - |
| 117 Arginine from beta-Alanine | Arginine | −beta-Alanine MCES +Urea | Transamination to Arginine using beta-Alanine | 2 Pyruvate(m) 4 beta-Alanine(s) 2 ATP-energy(c) 3 ATP-energy(m) 2 NADPH-redox-potential(m) 3 Proton-gradient(m) | 3 $CO_2$(s) 1 Pyruvate(c) 1 Arginine(s) 6 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 3 CoA-activated acetyl group(m) | 10 | 17 | - | - | - | - | - | - | 3 | - | 8 | - |
| 118 Asparagine from Alanine | Asparagine | −Alanine MCES +Urea | Transamination to Asparagine using Alanine | 1 Pyruvate(m) 2 Alanine(s) 2 ATP-energy(c) 1 ATP-energy(m) 1 NADPH-redox-potential(m) | 1 Pyruvate(c) 1 Asparagine(s) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 9 | 8 | - | - | - | - | - | - | 4 | - | 4 | - |
| 119 Asparagine from Arginine | Asparagine | −Arginine MCES +Urea | Transamination to Asparagine using Arginine | 3 $H_2O$(s) 0.5 $O_2$(s) 1 Arginine(s) 3 ATP-energy(c) | 1 $CO_2$(s) 1 Urea(s) 1 Asparagine(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 3 NADH-redox-potential(m) 4 Proton-gradient(m) | 9 | 10 | - | - | - | - | - | - | 6 | - | 12 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 120 Asparagine from Aspartate | Asparagine | −Aspartate MCES +Urea | Transamination to Asparagine using Aspartate | 2 Aspartate(s) 4 ATP-energy(c) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Asparagine(s) 1 NADPH-redox-potential(c) 2 Na-gradient(c) | 12 | - | - | - | - | - | - | - | 4 | - | - | - |
| 121 Asparagine from Cysteine | Asparagine | −Cysteine MCES +Urea +$H_2S$ | Transamination to Asparagine using Cysteine | 2 Pyruvate(m) 2 Cysteine(s) 3 ATP-energy(c) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 2 Pyruvate(c) 1 Asparagine(s) 2 $H_2S$(s) 1 NADH-redox-potential(m) 2 Na-gradient(c) 1 CoA-activated acetyl group(m) | 6 | 8 | - | - | - | - | - | - | 5 | - | 6 | - |
| 122 Asparagine from Cystine | Asparagine | −Cystine MCES +Urea +$H_2S$ | Transamination to Asparagine using Cystine | 2 Pyruvate(m) 1 Cystine(s) 3 ATP-energy(c) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 2 Pyruvate(c) 1 Asparagine(s) 2 $H_2S$(s) 1 NADH-redox-potential(m) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 8 | 8 | - | - | - | - | - | - | 5 | - | 6 | - |
| 123 Asparagine from Glutamate | Asparagine | −Glutamate MCES +Urea | Transamination to Asparagine using Glutamate | 2 $H_2O$(s) 1 $O_2$(s) 2 Glutamate(s) 3 ATP-energy(c) | 3 $CO_2$(s) 1 Pyruvate(m) 1 Asparagine(s) 2 ATP-energy(m) 3 NADH-redox-potential(m) 2 NADPH-redox-potential(m) 10 Proton-gradient(m) 2 Na-gradient(c) | 5 | 12 | - | - | - | - | - | - | 6 | - | 9 | - |
| 124 Asparagine from Glycine | Asparagine | −Glycine MCES +Urea | Transamination to Asparagine using Glycine | 2 Pyruvate(m) 2 Glycine(s) 3 ATP-energy(c) 2 NADPH-redox-potential(m) 2 Proton-gradient(m) 2 THF-activated methyl group(c) | 2 Pyruvate(c) 1 Asparagine(s) 2 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 10 | 8 | - | - | - | - | - | - | 3 | - | 6 | - |
| 125 Asparagine from Histidine | Asparagine | −Histidine MCES +Urea | Transamination to Asparagine using Histidine | 0.67 $H_2O$(s) 0.33 $O_2$(s) 0.33 Pyruvate(m) 0.67 Histidine(s) 3 ATP-energy(c) 0.67 NADPH-redox-potential(c) 0.33 NADPH-redox-potential(m) | 0.33 $CO_2$(s) 1 Asparagine(s) 0.67 ATP-energy(m) 0.33 NADH-redox-potential(c) 0.33 NADH-redox-potential(m) 3.67 Proton-gradient(m) 0.67 THF-activated methyl group(c) | 17 | 10 | - | - | - | - | - | - | 6 | - | 10 | - |
| 126 Asparagine from Isoleucine | Asparagine | −Isoleucine MCES +Urea | Transamination to Asparagine using Isoleucine | 2 $H_2O$(s) 2 $O_2$(s) 1 Pyruvate(m) 2 Isoleucine(s) 3 ATP-energy(c) 1 NADPH-redox-potential(m) | 3 $CO_2$(s) 1 Asparagine(s) 10 NADH-redox-potential(m) 20 Proton-gradient(m) 1 Na-gradient(c) 4 CoA-activated acetyl group(m) | 5 | 18 | - | - | - | - | - | - | 7 | - | 11 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 127 Asparagine from Glutamine | Asparagine | −Glutamine MCES +Urea | Transamination to Asparagine using Glutamine | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamine(s) 2 ATP-energy(c) | 1 $CO_2$(s) 1 Asparagine(s) 1 ATP-energy(m) 2 NADH-redox-potential(m) 5 Proton-gradient(m) | 4 | 9 | - | - | - | - | - | - | 5 | - | 7 | - |
| 128 Asparagine from Leucine | Asparagine | −Leucine MCES +Urea | Transamination to Asparagine using Leucine | 1 $O_2$(s) 2 Pyruvate(m) 2 Leucine(s) 3 ATP-energy(c) 3 NADPH-redox-potential(m) | 2 $H_2O$(s) 1 Asparagine(s) 7 NADH-redox-potential(m) 10 Proton-gradient(m) 2 Na-gradient(c) 7 CoA-activated acetyl group(m) | 5 | 16 | - | - | - | - | - | - | 5 | - | 10 | - |
| 129 Asparagine from Lysine | Asparagine | −Lysine MCES +Urea | Transamination to Asparagine using Lysine | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Pyruvate(m) 1 Lysine(s) 3 ATP-energy(c) 1 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Asparagine(s) 2 NADH-redox-potential(c) 3 NADH-redox-potential(m) 5 Proton-gradient(m) 2 CoA-activated acetyl group(m) | 9 | 13 | - | - | - | - | - | - | 4 | - | 12 | - |
| 130 Asparagine from Methionine | Asparagine | −Methionine MCES +Urea +$H_2S$ | Transamination to Asparagine using Methionine | 3 $H_2O$(s) 1 $O_2$(s) 1 Pyruvate(m) 2 Methionine(s) 1 Glucose-6P(c) 2 ATP-energy(c) 1 NADPH-redox-potential(m) | 1 $P_i$(c) 3 $CO_2$(s) 2 Pyruvate(c) 1 Asparagine(s) 2 $H_2S$(s) 5 NADH-redox-potential(c) 3 NADH-redox-potential(m) 5 Proton-gradient(m) 2 Na-gradient(c) 2 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 22 | 11 | - | - | - | - | - | - | 7 | - | 13 | - |
| 131 Asparagine from Phenylalanine | Asparagine | −Phenylalanine MCES +Urea | Transamination to Asparagine using Phenylalanine | 6 $O_2$(s) 2 Phenylalanine(s) 6 ATP-energy(c) 1 ATP-energy(m) 1 NADPH-redox-potential(c) 1 Proton-gradient(m) | 3 $CO_2$(s) 1 Pyruvate(c) 1 Asparagine(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 Na-gradient(c) 4 CoA-activated acetyl group(c) | 21 | 3 | - | - | - | - | - | - | 6 | - | 5 | - |
| 132 Asparagine from Proline | Asparagine | −Proline MCES +Urea | Transamination to Asparagine using Proline | 8 $H_2O$(s) 2 Proline(s) 3 ATP-energy(c) 1 Proton-gradient(m) | 3 $CO_2$(s) 1 Pyruvate(m) 1 Asparagine(s) 2 ATP-energy(m) 1 NADH-redox-potential(c) 4 NADH-redox-potential(m) 2 NADPH-redox-potential(m) | 8 | 13 | - | - | - | - | - | - | 4 | - | 7 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 133 Asparagine from Serine | Asparagine | −Serine MCES +Urea | Transamination to Asparagine using Serine | 2 Pyruvate(m) 2 Serine(s) 3 ATP-energy(c) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) | 2 $H_2O$(s) 2 Pyruvate(c) 1 Asparagine(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 2 Proton-gradient(c) 2 Na-gradient(c) 1 CoA-activated acetyl group(m) | 9 | 6 | - | - | - | - | - | - | 5 | - | 6 | - |
| 134 Asparagine from Threonine | Asparagine | −Threonine MCES +Urea | Transamination to Asparagine using Threonine | 1 $O_2$(s) 1 Pyruvate(m) 2 Threonine(s) 3 ATP-energy(c) 1 NADPH-redox-potential(m) | 3 $CO_2$(s) 1 Asparagine(s) 6 NADH-redox-potential(m) 8 Proton-gradient(m) 2 CoA-activated acetyl group(m) | 6 | 13 | - | - | - | - | - | - | 4 | - | 11 | - |
| 135 Asparagine from Tryptophan | Asparagine | −Tryptophan MCES +Urea | Transamination to Asparagine using Tryptophan | 3.5 $O_2$(s) 1 Pyruvate(m) 1 Tryptophan(s) 4 ATP-energy(c) 3 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 2 $CO_2$(s) 1 Pyruvate(c) 1 Asparagine(s) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 6 Proton-gradient(m) 1 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 23 | 9 | - | - | - | - | - | - | 4 | - | 7 | - |
| 136 Asparagine from Tyrosine | Asparagine | −Tyrosine MCES +Urea | Transamination to Asparagine using Tyrosine | 2 $H_2O$(s) 4 $O_2$(s) 2 Tyrosine(s) 6 ATP-energy(c) 1 ATP-energy(m) 1 Proton-gradient(m) | 3 $CO_2$(s) 1 Pyruvate(c) 1 Asparagine(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 2 Na-gradient(c) 4 CoA-activated acetyl group(c) | 19 | 3 | - | - | - | - | - | - | 7 | - | 5 | - |
| 137 Asparagine from Valine | Asparagine | −Valine MCES +Urea | Transamination to Asparagine using Valine | 4 $H_2O$(s) 2 $O_2$(s) 2 Valine(s) 3 ATP-energy(c) | 3 $CO_2$(s) 1 Pyruvate(m) 1 Asparagine(s) 2 ATP-energy(m) 1 NADH-redox-potential(c) 7 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 21 Proton-gradient(m) 1 Na-gradient(c) | 8 | 17 | - | - | - | - | - | - | 6 | - | 11 | - |
| 138 Asparagine from beta-Alanine | Asparagine | −beta-Alanine MCES +Urea | Transamination to Asparagine using beta-Alanine | 1 Pyruvate(m) 2 beta-Alanine(s) 3 ATP-energy(c) 2 Proton-gradient(m) | 1 $CO_2$(s) 1 Asparagine(s) 3 NADH-redox-potential(m) 2 CoA-activated acetyl group(m) | 5 | 8 | - | - | - | - | - | - | 3 | - | 8 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 139 Aspartate from Alanine | Aspartate | −Alanine MCES +Urea | Transamination to Aspartate using Alanine | 1 Pyruvate(m) 1 Alanine(s) 1 NADPH-redox-potential(c) | 1 Aspartate(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 6 | 3 | - | - | - | - | - | - | 2 | - | 1 | - |
| 140 Aspartate from Arginine | Aspartate | −Arginine MCES +Urea | Transamination to Aspartate using Arginine | 1.5 $H_2O$(s) 0.25 $O_2$(s) 0.5 Pyruvate(m) 0.5 Arginine(s) 0.5 NADPH-redox-potential(m) | 1 Aspartate(s) 0.5 Urea(s) 0.5 ATP-energy(m) 2 NADH-redox-potential(m) 0.5 Proton-gradient(m) | 1 | 13 | - | - | - | - | - | - | 5 | - | 10 | - |
| 141 Aspartate from Asparagine | Aspartate | −Asparagine MCES +Urea | Transamination to Aspartate using Asparagine | 1 Pyruvate(m) 0.5 Asparagine(s) 0.5 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 Aspartate(s) 0.5 NADH-redox-potential(m) 0.5 Proton-gradient(c) 0.5 Na-gradient(c) 0.5 CoA-activated acetyl group(m) | 1 | 8 | - | - | - | - | - | - | 4 | - | 6 | - |
| 142 Aspartate from Cysteine | Aspartate | −Cysteine MCES +Urea +$H_2S$ | Transamination to Aspartate using Cysteine | 2 Pyruvate(m) 1 Cysteine(s) 2 NADPH-redox-potential(m) 2 Proton-gradient(m) | 1 Pyruvate(c) 1 Aspartate(s) 1 $H_2S$(s) 2 NADH-redox-potential(m) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 1 | 8 | - | - | - | - | - | - | 4 | - | 6 | - |
| 143 Aspartate from Cystine | Aspartate | −Cystine MCES +Urea +$H_2S$ | Transamination to Aspartate using Cystine | 2 Pyruvate(m) 0.5 Cystine(s) 0.5 NADPH-redox-potential(c) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 Pyruvate(c) 1 Aspartate(s) 1 $H_2S$(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 0.5 Na-gradient(c) 1 CoA-activated acetyl group(m) | 6 | 6 | - | - | - | - | - | - | 5 | - | 6 | - |
| 144 Aspartate from Glutamate | Aspartate | −Glutamate MCES +Urea | Transamination to Aspartate using Glutamate | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamate(s) | 1 $CO_2$(s) 1 Aspartate(s) 1 ATP-energy(m) 2 NADH-redox-potential(m) 5 Proton-gradient(m) 1 Na-gradient(c) | - | 9 | - | - | - | - | - | - | 6 | - | 7 | - |
| 145 Aspartate from Glycine | Aspartate | −Glycine MCES +Urea | Transamination to Aspartate using Glycine | 2 Pyruvate(m) 1 Glycine(s) 2 NADPH-redox-potential(m) 2 Proton-gradient(m) 1 THF-activated methyl group(c) | 1 Pyruvate(c) 1 Aspartate(s) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 5 | 8 | - | - | - | - | - | - | 3 | - | 6 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 146 Aspartate from Histidine | Aspartate | −Histidine MCES +Urea | Transamination to Aspartate using Histidine | 0.33 $H_2O$(s) 0.17 $O_2$(s) 1 Pyruvate(m) 0.33 Histidine(s) 0.33 NADPH-redox-potential(c) 0.67 NADPH-redox-potential(m) | 1 Aspartate(s) 0.33 ATP-energy(m) 0.67 NADH-redox-potential(c) 0.33 Proton-gradient(c) 1.33 Proton-gradient(m) 0.33 Na-gradient(c) 0.33 THF-activated methyl group(c) 0.33 CoA-activated acetyl group(m) | 12 | 11 | - | - | - | - | - | - | 6 | - | 9 | - |
| 147 Aspartate from Isoleucine | Aspartate | −Isoleucine MCES +Urea | Transamination to Aspartate using Isoleucine | 1 $H_2O$(s) 1 $O_2$(s) 1 Pyruvate(m) 1 Isoleucine(s) 1 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Aspartate(s) 5 NADH-redox-potential(m) 9 Proton-gradient(m) 2 CoA-activated acetyl group(m) | - | 17 | - | - | - | - | - | - | 5 | - | 10 | - |
| 148 Aspartate from Glutamine | Aspartate | −Glutamine MCES +Urea | Transamination to Aspartate using Glutamine | 0.5 $H_2O$(s) 0.25 $O_2$(s) 0.5 Pyruvate(m) 0.5 Glutamine(s) 0.5 NADPH-redox-potential(m) | 1 Aspartate(s) 0.5 ATP-energy(m) 1 NADH-redox-potential(m) 1.5 Proton-gradient(m) | 2 | 12 | - | - | - | - | - | - | 4 | - | 8 | - |
| 149 Aspartate from Leucine | Aspartate | −Leucine MCES +Urea | Transamination to Aspartate using Leucine | 0.5 $O_2$(s) 2 Pyruvate(m) 1 Leucine(s) 2 NADPH-redox-potential(m) | 1 $H_2O$(s) 1 Aspartate(s) 4 NADH-redox-potential(m) 4 Proton-gradient(m) 1 Na-gradient(c) 4 CoA-activated acetyl group(m) | - | 15 | - | - | - | - | - | - | 5 | - | 9 | - |
| 150 Aspartate from Lysine | Aspartate | −Lysine MCES +Urea | Transamination to Aspartate using Lysine | 0.5 $H_2O$(s) 0.25 $O_2$(s) 1 Pyruvate(m) 0.5 Lysine(s) 1 NADPH-redox-potential(m) | 1 Aspartate(s) 0.5 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 2 | 14 | - | - | - | - | - | - | 4 | - | 9 | - |
| 151 Aspartate from Methionine | Aspartate | −Methionine MCES +Urea +$H_2S$ | Transamination to Aspartate using Methionine | 1.5 $H_2O$(s) 0.5 $O_2$(s) 1 Pyruvate(m) 1 Methionine(s) 0.5 Glucose-6P(c) 1 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Pyruvate(c) 1 Aspartate(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 16 | 13 | - | - | - | - | - | - | 7 | - | 13 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 152 Aspartate from Phenylalanine | Aspartate | −Phenylalanine MCES +Urea | Transamination to Aspartate using Phenylalanine | 3 $O_2$(s) 1 Phenylalanine(s) 2 ATP-energy(c) 1 NADPH-redox-potential(c) | 1 $CO_2$(s) 1 Aspartate(s) 1 NADH-redox-potential(c) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 18 | - | - | - | - | - | - | - | 5 | - | - | - |
| 153 Aspartate from Proline | Aspartate | −Proline MCES +Urea | Transamination to Aspartate using Proline | 4 $H_2O$(s) 1 Proline(s) | 1 $CO_2$(s) 1 Aspartate(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) | 3 | 10 | - | - | - | - | - | - | 4 | - | 4 | - |
| 154 Aspartate from Serine | Aspartate | −Serine MCES +Urea | Transamination to Aspartate using Serine | 2 Pyruvate(m) 1 Serine(s) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 $H_2O$(s) 1 Pyruvate(c) 1 Aspartate(s) 1 NADH-redox-potential(c) 1 Proton-gradient(c) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 4 | 5 | - | - | - | - | - | - | 5 | - | 6 | - |
| 155 Aspartate from Threonine | Aspartate | −Threonine MCES +Urea | Transamination to Aspartate using Threonine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 Threonine(s) 1 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Aspartate(s) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 4 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 4 | 11 | - | - | - | - | - | - | 4 | - | 10 | - |
| 156 Aspartate from Tryptophan | Aspartate | −Tryptophan MCES +Urea | Transamination to Aspartate using Tryptophan | 1.75 $O_2$(s) 1 Pyruvate(m) 0.5 Tryptophan(s) 0.5 ATP-energy(c) 1.5 NADPH-redox-potential(c) 1.5 NADPH-redox-potential(m) | 0.5 $CO_2$(s) 0.5 Pyruvate(c) 1 Aspartate(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 2.5 Proton-gradient(m) 0.5 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 19 | 10 | - | - | - | - | - | - | 4 | - | 10 | - |
| 157 Aspartate from Tyrosine | Aspartate | −Tyrosine MCES +Urea | Transamination to Aspartate using Tyrosine | 1 $H_2O$(s) 2 $O_2$(s) 1 Tyrosine(s) 2 ATP-energy(c) | 1 $CO_2$(s) 1 Aspartate(s) 1 NADH-redox-potential(c) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 15 | - | - | - | - | - | - | - | 6 | - | - | - |
| 158 Aspartate from Valine | Aspartate | −Valine MCES +Urea | Transamination to Aspartate using Valine | 2 $H_2O$(s) 1 $O_2$(s) 1 Valine(s) | 1 $CO_2$(s) 1 Aspartate(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 3 NADH-redox-potential(m) 10 Proton-gradient(m) 1 Na-gradient(c) | 3 | 14 | - | - | - | - | - | - | 6 | - | 10 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 159 Aspartate from beta-Alanine | Aspartate | −beta-Alanine MCES +Urea | Transamination to Aspartate using beta-Alanine | 1 Pyruvate(m) 1 beta-Alanine(s) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 1 Aspartate(s) 2 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | - | 8 | - | - | - | - | - | - | 2 | - | 5 | - |
| 160 Cysteine from Cystine | Cysteine | −Cystine MCES +Urea | Transamination to Cysteine using Cystine | 0.5 Cystine(s) 0.5 NADPH-redox-potential(c) | 1 Cysteine(s) 0.5 Na-gradient(c) | 2 | - | - | - | - | - | - | - | 4 | - | - | - |
| 161 Cysteine from Methionine | Cysteine | −Methionine MCES +Urea | Transamination to Cysteine using Methionine | 1.5 $H_2O$(s) 0.5 $O_2$(s) 1 Methionine(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Cysteine(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3 Proton-gradient(m) 2 Na-gradient(c) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 15 | 9 | - | - | - | - | - | - | 6 | - | 11 | - |
| 162 Cystine from Cysteine | Cystine | −Cysteine MCES +Urea | Transamination to Cystine using Cysteine | 2 Cysteine(s) | 1 Cystine(s) 1 NADPH-redox-potential(c) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 163 Cystine from Methionine | Cystine | −Methionine MCES +Urea | Transamination to Cystine using Methionine | 3 $H_2O$(s) 1 $O_2$(s) 2 Methionine(s) 1 Glucose-6P(c) | 1 $P_i$(c) 4 $CO_2$(s) 1 Cystine(s) 1 ATP-energy(c) 4 NADH-redox-potential(c) 4 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 6 Proton-gradient(m) 2 Na-gradient(c) 2 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 17 | 9 | - | - | - | - | - | - | 7 | - | 11 | - |
| 164 Glutamate from Alanine | Glutamate | −Alanine MCES +Urea | Transamination to Glutamate using Alanine | 1 $H_2O$(s) 1 Pyruvate(m) 1 Alanine(s) 1 ATP-energy(m) 1 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 1 Pyruvate(c) 1 Glutamate(s) 1 ATP-energy(c) 2 NADH-redox-potential(m) | 2 | 10 | - | - | - | - | - | - | 3 | - | 2 | - |
| 165 Glutamate from Arginine | Glutamate | −Arginine MCES +Urea | Transamination to Glutamate using Arginine | 1.5 $H_2O$(s) 0.5 Pyruvate(m) 0.5 Arginine(s) 0.5 NADPH-redox-potential(m) 1.5 Proton-gradient(m) 0.5 CoA-activated acetyl group(m) | 1 Glutamate(s) 0.5 Urea(s) 1.5 NADH-redox-potential(m) | 1 | 11 | - | - | - | - | - | - | 4 | - | 6 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 166 Glutamate from Asparagine | Glutamate | −Asparagine MCES +Urea | Transamination to Glutamate using Asparagine | 1 $H_2O$(s) 0.5 Pyruvate(m) 0.5 Asparagine(s) 0.5 NADH-redox-potential(c) 1 NADPH-redox-potential(m) 0.5 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 0.5 $CO_2$(s) 1 Glutamate(s) 1.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 0.5 Proton-gradient(c) 0.5 Na-gradient(c) | 7 | 10 | - | - | - | - | - | - | 6 | - | 6 | - |
| 167 Glutamate from Aspartate | Glutamate | −Aspartate MCES +Urea | Transamination to Glutamate using Aspartate | 1 $H_2O$(s) 1 Aspartate(s) 1 NADH-redox-potential(c) 1 CoA-activated acetyl group(m) | 1 $CO_2$(s) 1 Glutamate(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 6 | 5 | - | - | - | - | - | - | 5 | - | 2 | - |
| 168 Glutamate from Cysteine | Glutamate | −Cysteine MCES +Urea +$H_2S$ | Transamination to Glutamate using Cysteine | 1 $H_2O$(s) 1 Pyruvate(m) 1 Cysteine(s) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 Pyruvate(c) 1 Glutamate(s) 1 $H_2S$(s) 1 NADH-redox-potential(m) 1 Na-gradient(c) | 1 | 10 | - | - | - | - | - | - | 5 | - | 4 | - |
| 169 Glutamate from Cystine | Glutamate | −Cystine MCES +Urea +$H_2S$ | Transamination to Glutamate using Cystine | 1 $H_2O$(s) 1 Pyruvate(m) 0.5 Cystine(s) 0.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 Pyruvate(c) 1 Glutamate(s) 1 $H_2S$(s) 1 NADH-redox-potential(m) | 3 | 10 | - | - | - | - | - | - | 4 | - | 4 | - |
| 170 Glutamate from Glycine | Glutamate | −Glycine MCES +Urea | Transamination to Glutamate using Glycine | 1 $H_2O$(s) 1 Pyruvate(m) 1 Glycine(s) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 1 Pyruvate(c) 1 Glutamate(s) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 5 | 10 | - | - | - | - | - | - | 4 | - | 4 | - |
| 171 Glutamate from Histidine | Glutamate | −Histidine MCES +Urea | Transamination to Glutamate using Histidine | 0.67 $H_2O$(s) 0.67 Pyruvate(m) 0.33 Histidine(s) 0.33 NADH-redox-potential(c) 0.33 NADPH-redox-potential(c) 0.67 NADPH-redox-potential(m) 0.67 Proton-gradient(m) 0.67 CoA-activated acetyl group(m) | 1 Glutamate(s) 0.67 NADH-redox-potential(m) 0.33 Na-gradient(c) 0.33 THF-activated methyl group(c) | 10 | 10 | - | - | - | - | - | - | 4 | - | 4 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 172 Glutamate from Isoleucine | Glutamate | −Isoleucine MCES +Urea | Transamination to Glutamate using Isoleucine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 Isoleucine(s) 1 NADPH-redox-potential(m) | 1 Glutamate(s) 3 NADH-redox-potential(m) 4 Proton-gradient(m) 2 CoA-activated acetyl group(m) | - | 17 | - | - | - | - | - | - | 3 | - | 7 | - |
| 173 Glutamate from Glutamine | Glutamate | −Glutamine MCES +Urea | Transamination to Glutamate using Glutamine | 0.5 $H_2O$(s) 0.5 Pyruvate(m) 0.5 Glutamine(s) 1 NADPH-redox-potential(m) 0.5 Proton-gradient(m) 0.5 CoA-activated acetyl group(m) | 1 Glutamate(s) 1 NADH-redox-potential(m) | 2 | 10 | - | - | - | - | - | - | 3 | - | 4 | - |
| 174 Glutamate from Leucine | Glutamate | −Leucine MCES +Urea | Transamination to Glutamate using Leucine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 Leucine(s) 2 NADPH-redox-potential(m) | 1 Glutamate(s) 4 NADH-redox-potential(m) 5 Proton-gradient(m) 1 Na-gradient(c) 2 CoA-activated acetyl group(m) | - | 17 | - | - | - | - | - | - | 4 | - | 7 | - |
| 175 Glutamate from Lysine | Glutamate | −Lysine MCES +Urea | Transamination to Glutamate using Lysine | 1.5 $H_2O$(s) 0.25 $O_2$(s) 1 Pyruvate(m) 0.5 Lysine(s) 1 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Glutamate(s) 0.5 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 2 Proton-gradient(m) | 6 | 13 | - | - | - | - | - | - | 5 | - | 10 | - |
| 176 Glutamate from Methionine | Glutamate | −Methionine MCES +Urea +$H_2S$ | Transamination to Glutamate using Methionine | 0.5 $H_2O$(s) 1 Pyruvate(m) 1 Methionine(s) 0.5 Glucose-6P(c) 1 NADPH-redox-potential(m) 4 Proton-gradient(m) | 0.5 $P_i$(c) 1 Pyruvate(c) 1 Glutamate(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 Na-gradient(c) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 16 | 12 | - | - | - | - | - | - | 5 | - | 8 | - |
| 177 Glutamate from Phenylalanine | Glutamate | −Phenylalanine MCES +Urea | Transamination to Glutamate using Phenylalanine | 1 $H_2O$(s) 3 $O_2$(s) 1 Phenylalanine(s) 2 ATP-energy(c) 1 CoA-activated acetyl group(m) | 2 $CO_2$(s) 1 Glutamate(s) 1 NADH-redox-potential(m) 2 CoA-activated acetyl group(c) | 17 | 4 | - | - | - | - | - | - | 5 | - | 2 | - |
| 178 Glutamate from Proline | Glutamate | −Proline MCES +Urea | Transamination to Glutamate using Proline | 2 $H_2O$(s) 1 Proline(s) | 1 Glutamate(s) 4 Proton-gradient(m) | - | 3 | - | - | - | - | - | - | 3 | - | 4 | - |
| 179 Glutamate from Serine | Glutamate | −Serine MCES +Urea | Transamination to Glutamate using Serine | 1 Pyruvate(m) 1 Serine(s) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 Pyruvate(c) 1 Glutamate(s) 2 NADH-redox-potential(m) 1 Proton-gradient(c) 1 Na-gradient(c) | 1 | 10 | - | - | - | - | - | - | 4 | - | 4 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 180 Glutamate from Threonine | Glutamate | −Threonine MCES +Urea | Transamination to Glutamate using Threonine | 0.17 $O_2$(s) 0.33 Pyruvate(m) 1 Threonine(s) 1 NADPH-redox-potential(m) | 0.33 $H_2O$(s) 1 Glutamate(s) 1.33 NADH-redox-potential(m) | 1 | 20 | - | - | - | - | - | - | 4 | - | 8 | - |
| 181 Glutamate from Tryptophan | Glutamate | −Tryptophan MCES +Urea | Transamination to Glutamate using Tryptophan | 1 $H_2O$(s) 1.75 $O_2$(s) 1 Pyruvate(m) 0.5 Tryptophan(s) 0.5 ATP-energy(c) 0.5 NADPH-redox-potential(c) 1.5 NADPH-redox-potential(m) | 1.5 $CO_2$(s) 0.5 Pyruvate(c) 1 Glutamate(s) 2 NADH-redox-potential(m) 2.5 Proton-gradient(m) 0.5 THF-activated methyl group(c) | 19 | 11 | - | - | - | - | - | - | 5 | - | 10 | - |
| 182 Glutamate from Tyrosine | Glutamate | −Tyrosine MCES +Urea | Transamination to Glutamate using Tyrosine | 2 $H_2O$(s) 2 $O_2$(s) 1 Tyrosine(s) 2 ATP-energy(c) 1 CoA-activated acetyl group(m) | 2 $CO_2$(s) 1 Glutamate(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 16 | 4 | - | - | - | - | - | - | 6 | - | 2 | - |
| 183 Glutamate from Valine | Glutamate | −Valine MCES +Urea | Transamination to Glutamate using Valine | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Valine(s) | 1 Glutamate(s) 2 NADH-redox-potential(m) 4 Proton-gradient(m) 1 Na-gradient(c) | - | 10 | - | - | - | - | - | - | 5 | - | 8 | - |
| 184 Glutamate from beta-Alanine | Glutamate | −beta-Alanine MCES +Urea | Transamination to Glutamate using beta-Alanine | 1 $H_2O$(s) 1 Pyruvate(m) 1 beta-Alanine(s) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 $CO_2$(s) 1 Glutamate(s) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) | 3 | 8 | - | - | - | - | - | - | 4 | - | 6 | - |
| 185 Glycine from Alanine | Glycine | −Alanine MCES +Urea | Transamination to Glycine using Alanine | 0.5 $H_2O$(s) 1 Alanine(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 1 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 1 NADH-redox-potential(c) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 15 | - | - | - | - | - | - | - | 3 | - | - | - |
| 186 Glycine from Arginine | Glycine | −Arginine MCES +Urea | Transamination to Glycine using Arginine | 2 $H_2O$(s) 0.25 $O_2$(s) 0.5 Arginine(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 1 $CO_2$(s) 0.5 Pyruvate(c) 1 Glycine(s) 0.5 Urea(s) 0.5 ATP-energy(c) 0.5 ATP-energy(m) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 1 Proton-gradient(m) 1 THF-activated methyl group(c) | 17 | 9 | - | - | - | - | - | - | 6 | - | 13 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 187 Glycine from Asparagine | Glycine | −Asparagine MCES +Urea | Transamination to Glycine using Asparagine | 0.5 $H_2O$(s) 0.5 Glucose-6P(c) 0.5 Asparagine(s) 0.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) 1 Proton-gradient(m) | 0.5 $P_i$(c) 0.5 $CO_2$(s) 0.5 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 1.5 NADH-redox-potential(c) 0.5 Na-gradient(c) 1 THF-activated methyl group(c) | 19 | 2 | - | - | - | - | - | - | 5 | - | 7 | - |
| 188 Glycine from Aspartate | Glycine | −Aspartate MCES +Urea | Transamination to Glycine using Aspartate | 0.5 $H_2O$(s) 1 Aspartate(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 1 NADPH-redox-potential(c) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 17 | - | - | - | - | - | - | - | 5 | - | - | - |
| 189 Glycine from Cysteine | Glycine | −Cysteine MCES +Urea +$H_2S$ | Transamination to Glycine using Cysteine | 0.5 $H_2O$(s) 0.5 Glucose-6P(c) 1 Cysteine(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 2 Proton-gradient(m) | 0.5 $P_i$(c) 1 Pyruvate(c) 1 Glycine(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 16 | 2 | - | - | - | - | - | - | 4 | - | 7 | - |
| 190 Glycine from Cystine | Glycine | −Cystine MCES +Urea +$H_2S$ | Transamination to Glycine using Cystine | 0.5 $H_2O$(s) 0.5 Glucose-6P(c) 0.5 Cystine(s) 1 NADH-redox-potential(m) 1.5 NADPH-redox-potential(c) 2 Proton-gradient(m) | 0.5 $P_i$(c) 1 Pyruvate(c) 1 Glycine(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 0.5 Na-gradient(c) 1 THF-activated methyl group(c) | 17 | 2 | - | - | - | - | - | - | 6 | - | 7 | - |
| 191 Glycine from Glutamate | Glycine | −Glutamate MCES +Urea | Transamination to Glycine using Glutamate | 1.5 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamate(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 1 ATP-energy(m) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 6 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 16 | 7 | - | - | - | - | - | - | 6 | - | 7 | - |
| 192 Glycine from Histidine | Glycine | −Histidine MCES +Urea | Transamination to Glycine using Histidine | 0.83 $H_2O$(s) 0.17 $O_2$(s) 0.5 Glucose-6P(c) 0.33 Histidine(s) 0.33 NADH-redox-potential(m) | 0.5 $P_i$(c) 0.67 $CO_2$(s) 0.33 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 0.33 ATP-energy(m) 0.67 NADH-redox-potential(c) 0.67 Proton-gradient(m) 1.33 THF-activated methyl group(c) | 21 | 8 | - | - | - | - | - | - | 5 | - | 12 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 193 Glycine from Isoleucine | Glycine | −Isoleucine MCES +Urea | Transamination to Glycine using Isoleucine | 1.5 $H_2O$(s) 1 $O_2$(s) 0.5 Glucose-6P(c) 1 Isoleucine(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Glycine(s) 0.5 ATP-energy(c) 1 NADH-redox-potential(c) 4 NADH-redox-potential(m) 9 Proton-gradient(m) 1 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 14 | 13 | - | - | - | - | - | - | 4 | - | 11 | - |
| 194 Glycine from Glutamine | Glycine | −Glutamine MCES +Urea | Transamination to Glycine using Glutamine | 1 $H_2O$(s) 0.25 $O_2$(s) 0.5 Glutamine(s) 0.5 Glucose-6P(c) 0.5 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 0.5 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 0.5 ATP-energy(m) 1 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 2 Proton-gradient(m) 1 THF-activated methyl group(c) | 18 | 9 | - | - | - | - | - | - | 5 | - | 11 | - |
| 195 Glycine from Leucine | Glycine | −Leucine MCES +Urea | Transamination to Glycine using Leucine | 0.5 $O_2$(s) 0.5 Glucose-6P(c) 1 Leucine(s) 1 NADPH-redox-potential(m) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 Glycine(s) 0.5 ATP-energy(c) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 4 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) 3 CoA-activated acetyl group(m) | 14 | 13 | - | - | - | - | - | - | 4 | - | 10 | - |
| 196 Glycine from Lysine | Glycine | −Lysine MCES +Urea | Transamination to Glycine using Lysine | 1 $H_2O$(s) 0.25 $O_2$(s) 0.5 Lysine(s) 0.5 Glucose-6P(c) 0.5 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Glycine(s) 0.5 ATP-energy(c) 1.5 NADH-redox-potential(c) 1.5 NADH-redox-potential(m) 1 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 15 | 11 | - | - | - | - | - | - | 5 | - | 11 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 197 Glycine from Methionine | Glycine | −Methionine MCES +Urea +$H_2S$ | Transamination to Glycine using Methionine | 2 $H_2O$(s) 0.5 $O_2$(s) 1 Methionine(s) 1 Glucose-6P(c) 1 NADPH-redox-potential(c) | 1 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Glycine(s) 1 $H_2S$(s) 1 ATP-energy(c) 4 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 Proton-gradient(m) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 19 | 9 | - | - | - | - | - | - | 5 | - | 12 | - |
| 198 Glycine from Phenylalanine | Glycine | −Phenylalanine MCES +Urea | Transamination to Glycine using Phenylalanine | 0.5 $H_2O$(s) 3 $O_2$(s) 1 Phenylalanine(s) 0.5 Glucose-6P(c) 1.5 ATP-energy(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Glycine(s) 1 NADH-redox-potential(c) 1 THF-activated methyl group(c) 2 CoA-activated acetyl group(c) | 28 | - | - | - | - | - | - | - | 4 | - | - | - |
| 199 Glycine from Proline | Glycine | −Proline MCES +Urea | Transamination to Glycine using Proline | 4.5 $H_2O$(s) 0.5 Glucose-6P(c) 1 Proline(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 1 ATP-energy(m) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 16 | 10 | - | - | - | - | - | - | 3 | - | 4 | - |
| 200 Glycine from Serine | Glycine | −Serine MCES +Urea | Transamination to Glycine using Serine | 1 Serine(s) 1 NADH-redox-potential(c) | 1 $H_2O$(s) 1 Glycine(s) 1 THF-activated methyl group(c) | 4 | - | - | - | - | - | - | - | 2 | - | - | - |
| 201 Glycine from Threonine | Glycine | −Threonine MCES +Urea | Transamination to Glycine using Threonine | 0.5 $H_2O$(s) 0.5 $O_2$(s) 0.5 Glucose-6P(c) 1 Threonine(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Glycine(s) 0.5 ATP-energy(c) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 15 | 9 | - | - | - | - | - | - | 4 | - | 11 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 202 Glycine from Tryptophan | Glycine | −Tryptophan MCES +Urea | Transamination to Glycine using Tryptophan | 0.5 $H_2O$(s) 1.75 $O_2$(s) 0.5 Tryptophan(s) 0.5 Glucose-6P(c) 1.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1.5 $CO_2$(s) 0.5 Pyruvate(c) 1 Glycine(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1.5 Proton-gradient(m) 0.5 Na-gradient(c) 1.5 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 26 | 9 | - | - | - | - | - | - | 6 | - | 12 | - |
| 203 Glycine from Tyrosine | Glycine | −Tyrosine MCES +Urea | Transamination to Glycine using Tyrosine | 1.5 $H_2O$(s) 2 $O_2$(s) 1 Tyrosine(s) 0.5 Glucose-6P(c) 1.5 ATP-energy(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Glycine(s) 2 NADH-redox-potential(c) 1 THF-activated methyl group(c) 2 CoA-activated acetyl group(c) | 26 | - | - | - | - | - | - | - | 4 | - | - | - |
| 204 Glycine from Valine | Glycine | −Valine MCES +Urea | Transamination to Glycine using Valine | 2.5 $H_2O$(s) 1 $O_2$(s) 0.5 Glucose-6P(c) 1 Valine(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Glycine(s) 0.5 ATP-energy(c) 1 ATP-energy(m) 2 NADH-redox-potential(c) 3 NADH-redox-potential(m) 10 Proton-gradient(m) 1 THF-activated methyl group(c) | 15 | 14 | - | - | - | - | - | - | 4 | - | 10 | - |
| 205 Glycine from beta-Alanine | Glycine | −beta-Alanine MCES +Urea | Transamination to Glycine using beta-Alanine | 0.5 $H_2O$(s) 0.5 Glucose-6P(c) 1 beta-Alanine(s) 1 NADPH-redox-potential(c) 2 Proton-gradient(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Glycine(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 15 | 4 | - | - | - | - | - | - | 4 | - | 7 | - |
| 206 Glutamine from Alanine | Glutamine | −Alanine MCES +Urea | Transamination to Glutamine using Alanine | 1 $H_2O$(s) 2 Alanine(s) 1 ATP-energy(m) 1 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 1 Pyruvate(c) 1 Glutamine(s) 3 NADH-redox-potential(m) | 2 | 12 | - | - | - | - | - | - | 3 | - | 5 | - |
| 207 Glutamine from Arginine | Glutamine | −Arginine MCES +Urea | Transamination to Glutamine using Arginine | 2 $H_2O$(s) 1 Arginine(s) 1 ATP-energy(c) 2 Proton-gradient(m) | 1 Glutamine(s) 1 Urea(s) 2 NADH-redox-potential(m) | 3 | 4 | - | - | - | - | - | - | 4 | - | 7 | - |
| 208 Glutamine from Asparagine | Glutamine | −Asparagine MCES +Urea | Transamination to Glutamine using Asparagine | 1 $H_2O$(s) 1 Asparagine(s) 1 ATP-energy(c) 1 NADH-redox-potential(c) 1 CoA-activated acetyl group(m) | 1 $CO_2$(s) 1 Glutamine(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) | 9 | 5 | - | - | - | - | - | - | 4 | - | 2 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 209 Glutamine from Aspartate | Glutamine | −Aspartate MCES +Urea | Transamination to Glutamine using Aspartate | 1 $H_2O$(s) 2 Aspartate(s) 2 ATP-energy(c) 1 NADH-redox-potential(c) 1 CoA-activated acetyl group(m) | 2 $CO_2$(s) 1 Pyruvate(c) 1 Glutamine(s) 1 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 2 Na-gradient(c) | 14 | 5 | - | - | - | - | - | - | 5 | - | 2 | - |
| 210 Glutamine from Cysteine | Glutamine | −Cysteine MCES +Urea +$H_2S$ | Transamination to Glutamine using Cysteine | 1 $H_2O$(s) 1 Pyruvate(m) 2 Cysteine(s) 1 ATP-energy(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 2 Pyruvate(c) 1 Glutamine(s) 2 $H_2S$(s) 1 NADH-redox-potential(m) 2 Na-gradient(c) | 3 | 10 | - | - | - | - | - | - | 6 | - | 4 | - |
| 211 Glutamine from Cystine | Glutamine | −Cystine MCES +Urea +$H_2S$ | Transamination to Glutamine using Cystine | 1 $H_2O$(s) 1 Pyruvate(m) 1 Cystine(s) 1 ATP-energy(c) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 2 Pyruvate(c) 1 Glutamine(s) 2 $H_2S$(s) 1 NADH-redox-potential(m) 1 Na-gradient(c) | 5 | 10 | - | - | - | - | - | - | 6 | - | 4 | - |
| 212 Glutamine from Glutamate | Glutamine | −Glutamate MCES +Urea | Transamination to Glutamine using Glutamate | 1 $H_2O$(s) 0.5 $O_2$(s) 2 Glutamate(s) 1 ATP-energy(c) | 2 $CO_2$(s) 1 Pyruvate(m) 1 Glutamine(s) 1 ATP-energy(m) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 5 Proton-gradient(m) 2 Na-gradient(c) | 2 | 10 | - | - | - | - | - | - | 6 | - | 8 | - |
| 213 Glutamine from Glycine | Glutamine | −Glycine MCES +Urea | Transamination to Glutamine using Glycine | 1 $H_2O$(s) 1 Pyruvate(m) 2 Glycine(s) 1 ATP-energy(c) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 2 Pyruvate(c) 1 Glutamine(s) 2 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 2 Na-gradient(c) | 7 | 10 | - | - | - | - | - | - | 4 | - | 4 | - |
| 214 Glutamine from Histidine | Glutamine | −Histidine MCES +Urea | Transamination to Glutamine using Histidine | 0.33 $H_2O$(s) 0.33 Pyruvate(m) 0.67 Histidine(s) 1 ATP-energy(c) 0.67 NADH-redox-potential(c) 0.67 NADPH-redox-potential(c) 0.33 NADPH-redox-potential(m) 0.33 Proton-gradient(m) 0.33 CoA-activated acetyl group(m) | 1 Glutamine(s) 0.33 NADH-redox-potential(m) 0.67 THF-activated methyl group(c) | 12 | 10 | - | - | - | - | - | - | 4 | - | 4 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 215 Glutamine from Isoleucine | Glutamine | −Isoleucine MCES +Urea | Transamination to Glutamine using Isoleucine | 1 $H_2O$(s) 1.5 $O_2$(s) 2 Isoleucine(s) 1 ATP-energy(c) 1 ATP-energy(m) | 1 $CO_2$(s) 1 Glutamine(s) 6 NADH-redox-potential(m) 15 Proton-gradient(m) 3 CoA-activated acetyl group(m) | 4 | 19 | - | - | - | - | - | - | 6 | - | 11 | - |
| 216 Glutamine from Leucine | Glutamine | −Leucine MCES +Urea | Transamination to Glutamine using Leucine | 1 $O_2$(s) 1 Pyruvate(m) 2 Leucine(s) 1 ATP-energy(c) 3 NADPH-redox-potential(m) | 1 $H_2O$(s) 1 Glutamine(s) 7 NADH-redox-potential(m) 11 Proton-gradient(m) 2 Na-gradient(c) 5 CoA-activated acetyl group(m) | 2 | 18 | - | - | - | - | - | - | 6 | - | 8 | - |
| 217 Glutamine from Lysine | Glutamine | −Lysine MCES +Urea | Transamination to Glutamine using Lysine | 2 $H_2O$(s) 0.5 $O_2$(s) 1 Pyruvate(m) 1 Lysine(s) 1 ATP-energy(c) 1 NADPH-redox-potential(m) | 2 $CO_2$(s) 1 Glutamine(s) 1 NADH-redox-potential(c) 5 NADH-redox-potential(m) 5 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 4 | 18 | - | - | - | - | - | - | 4 | - | 11 | - |
| 218 Glutamine from Methionine | Glutamine | −Methionine MCES +Urea +$H_2S$ | Transamination to Glutamine using Methionine | 2 $H_2O$(s) 0.5 $O_2$(s) 2 Methionine(s) 1 Glucose-6P(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 1 Glutamine(s) 2 $H_2S$(s) 4 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 Na-gradient(c) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 16 | 17 | - | - | - | - | - | - | 8 | - | 12 | - |
| 219 Glutamine from Phenylalanine | Glutamine | −Phenylalanine MCES +Urea | Transamination to Glutamine using Phenylalanine | 1 $H_2O$(s) 6 $O_2$(s) 2 Phenylalanine(s) 4 ATP-energy(c) 1 ATP-energy(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 4 $CO_2$(s) 1 Pyruvate(c) 1 Glutamine(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 1 Na-gradient(c) 4 CoA-activated acetyl group(c) | 19 | 7 | - | - | - | - | - | - | 7 | - | 7 | - |
| 220 Glutamine from Proline | Glutamine | −Proline MCES +Urea | Transamination to Glutamine using Proline | 6 $H_2O$(s) 2 Proline(s) 1 ATP-energy(c) | 2 $CO_2$(s) 1 Pyruvate(m) 1 Glutamine(s) 1 ATP-energy(m) 2 NADH-redox-potential(m) 2 NADPH-redox-potential(m) 3 Proton-gradient(m) 1 Na-gradient(c) | 2 | 13 | - | - | - | - | - | - | 6 | - | 7 | - |
| 221 Glutamine from Serine | Glutamine | −Serine MCES +Urea | Transamination to Glutamine using Serine | 1 Pyruvate(m) 2 Serine(s) 1 ATP-energy(c) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 $H_2O$(s) 2 Pyruvate(c) 1 Glutamine(s) 2 NADH-redox-potential(m) 1 Proton-gradient(c) 1 Na-gradient(c) | 3 | 10 | - | - | - | - | - | - | 5 | - | 4 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 222 Glutamine from Threonine | Glutamine | −Threonine MCES +Urea | Transamination to Glutamine using Threonine | 0.5 $O_2$(s) 2 Threonine(s) 1 ATP-energy(c) 1 NADPH-redox-potential(m) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Glutamine(s) 3 NADH-redox-potential(m) 3 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 3 | 17 | - | - | - | - | - | - | 6 | - | 9 | - |
| 223 Glutamine from Tryptophan | Glutamine | −Tryptophan MCES +Urea | Transamination to Glutamine using Tryptophan | 1 $H_2O$(s) 3.5 $O_2$(s) 1 Pyruvate(m) 1 Tryptophan(s) 2 ATP-energy(c) 2 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 3 $CO_2$(s) 1 Pyruvate(c) 1 Glutamine(s) 3 NADH-redox-potential(m) 6 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 20 | 11 | - | - | - | - | - | - | 6 | - | 8 | - |
| 224 Glutamine from Tyrosine | Glutamine | −Tyrosine MCES +Urea | Transamination to Glutamine using Tyrosine | 3 $H_2O$(s) 4 $O_2$(s) 2 Tyrosine(s) 4 ATP-energy(c) 1 ATP-energy(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 4 $CO_2$(s) 1 Pyruvate(c) 1 Glutamine(s) 2 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 2 Na-gradient(c) 4 CoA-activated acetyl group(c) | 18 | 6 | - | - | - | - | - | - | 7 | - | 7 | - |
| 225 Glutamine from Valine | Glutamine | −Valine MCES +Urea | Transamination to Glutamine using Valine | 3 $H_2O$(s) 1.5 $O_2$(s) 2 Valine(s) | 2 $CO_2$(s) 1 Pyruvate(c) 1 Glutamine(s) 6 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 15 Proton-gradient(m) 2 Na-gradient(c) | 4 | 14 | - | - | - | - | - | - | 7 | - | 13 | - |
| 226 Glutamine from beta-Alanine | Glutamine | −beta-Alanine MCES +Urea | Transamination to Glutamine using beta-Alanine | 1 $H_2O$(s) 1 Pyruvate(m) 2 beta-Alanine(s) 1 ATP-energy(c) 1 Proton-gradient(m) | 2 $CO_2$(s) 1 Glutamine(s) 3 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(m) | 5 | 9 | - | - | - | - | - | - | 4 | - | 8 | - |
| 227 Methionine from Cysteine | Methionine | −Cysteine MCES +Urea | Transamination to Methionine using Cysteine | 1 $H_2O$(s) 1 Pyruvate(m) 1 Cysteine(s) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Methionine(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 8 | 12 | - | - | - | - | - | - | 5 | - | 4 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 228 Methionine from Cystine | Methionine | −Cystine MCES +Urea | Transamination to Methionine using Cystine | 1 $H_2O$(s) 1 Pyruvate(m) 0.5 Cystine(s) 0.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Methionine(s) 2 NADH-redox-potential(m) 0.5 Na-gradient(c) | 7 | 14 | - | - | - | - | - | - | 6 | - | 4 | - |
| 229 Proline from Alanine | Proline | −Alanine MCES +Urea | Transamination to Proline using Alanine | 0.5 $O_2$(s) 1 Alanine(s) 1 ATP-energy(m) 2 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 2 $H_2O$(s) 1 Proline(s) 2 NADH-redox-potential(m) 5 Proton-gradient(m) 1 Na-gradient(c) | - | 15 | - | - | - | - | - | - | 5 | - | 7 | - |
| 230 Proline from Arginine | Proline | −Arginine MCES +Urea | Transamination to Proline using Arginine | 0.5 $O_2$(s) 0.5 Pyruvate(m) 0.5 Arginine(s) 0.5 ATP-energy(m) 1 NADPH-redox-potential(m) 0.5 CoA-activated acetyl group(m) | 1.5 $H_2O$(s) 0.5 Urea(s) 1 Proline(s) 1 NADH-redox-potential(m) 4.5 Proton-gradient(m) | 1 | 15 | - | - | - | - | - | - | 6 | - | 8 | - |
| 231 Proline from Asparagine | Proline | −Asparagine MCES +Urea | Transamination to Proline using Asparagine | 0.5 $O_2$(s) 0.5 Pyruvate(m) 0.5 Asparagine(s) 1 ATP-energy(m) 0.5 NADH-redox-potential(c) 2 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 2 $H_2O$(s) 0.5 $CO_2$(s) 1 Proline(s) 1.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 5.5 Proton-gradient(m) | 7 | 15 | - | - | - | - | - | - | 5 | - | 9 | - |
| 232 Proline from Aspartate | Proline | −Aspartate MCES +Urea | Transamination to Proline using Aspartate | 0.5 $O_2$(s) 1 Aspartate(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 2 $H_2O$(s) 1 $CO_2$(s) 1 Proline(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 6 Proton-gradient(m) 1 Na-gradient(c) | 6 | 11 | - | - | - | - | - | - | 6 | - | 7 | - |
| 233 Proline from Cysteine | Proline | −Cysteine MCES +Urea +$H_2S$ | Transamination to Proline using Cysteine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 Cysteine(s) 1 ATP-energy(m) 2 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 2 $H_2O$(s) 1 Pyruvate(c) 1 Proline(s) 1 $H_2S$(s) 1 NADH-redox-potential(m) 5 Proton-gradient(m) | 1 | 15 | - | - | - | - | - | - | 5 | - | 7 | - |
| 234 Proline from Cystine | Proline | −Cystine MCES +Urea +$H_2S$ | Transamination to Proline using Cystine | 0.5 $O_2$(s) 1 Pyruvate(m) 0.5 Cystine(s) 1 ATP-energy(m) 0.5 NADPH-redox-potential(c) 3 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 2 $H_2O$(s) 1 Pyruvate(c) 1 Proline(s) 1 $H_2S$(s) 2 NADH-redox-potential(m) 5 Proton-gradient(m) 0.5 Na-gradient(c) | 3 | 15 | - | - | - | - | - | - | 7 | - | 7 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 235 Proline from Glutamate | Proline | −Glutamate MCES +Urea | Transamination to Proline using Glutamate | 0.5 $O_2$(s) 1 Glutamate(s) 1 NADH-redox-potential(m) | 3 $H_2O$(s) 1 Proline(s) 6 Proton-gradient(m) 1 Na-gradient(c) | - | 4 | - | - | - | - | - | - | 5 | - | 6 | - |
| 236 Proline from Glycine | Proline | −Glycine MCES +Urea | Transamination to Proline using Glycine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 Glycine(s) 1 ATP-energy(m) 3 NADPH-redox-potential(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 2 $H_2O$(s) 1 Pyruvate(c) 1 Proline(s) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 5 Proton-gradient(m) 1 Na-gradient(c) | 5 | 15 | - | - | - | - | - | - | 4 | - | 7 | - |
| 237 Proline from Histidine | Proline | −Histidine MCES +Urea | Transamination to Proline using Histidine | 0.5 $O_2$(s) 0.67 Pyruvate(m) 0.33 Histidine(s) 1 ATP-energy(m) 1.67 NADPH-redox-potential(m) 0.67 CoA-activated acetyl group(m) | 1.67 $H_2O$(s) 0.33 $CO_2$(s) 1 Proline(s) 0.67 NADH-redox-potential(m) 0.33 NADPH-redox-potential(c) 5.33 Proton-gradient(m) 0.33 Na-gradient(c) | 8 | 15 | - | - | - | - | - | - | 7 | - | 8 | - |
| 238 Proline from Isoleucine | Proline | −Isoleucine MCES +Urea | Transamination to Proline using Isoleucine | 1.17 $O_2$(s) 0.33 Pyruvate(m) 1 Isoleucine(s) 1 ATP-energy(m) 2 NADPH-redox-potential(m) | 2.33 $H_2O$(s) 1 Proline(s) 3.33 NADH-redox-potential(m) 12 Proton-gradient(m) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | - | 30 | - | - | - | - | - | - | 5 | - | 7 | - |
| 239 Proline from Glutamine | Proline | −Glutamine MCES +Urea | Transamination to Proline using Glutamine | 0.5 $O_2$(s) 0.5 Pyruvate(m) 0.5 Glutamine(s) 1 ATP-energy(m) 2 NADPH-redox-potential(m) 0.5 CoA-activated acetyl group(m) | 2.5 $H_2O$(s) 1 Proline(s) 1 NADH-redox-potential(m) 5 Proton-gradient(m) 0.5 Na-gradient(c) | - | 16 | - | - | - | - | - | - | 6 | - | 7 | - |
| 240 Proline from Leucine | Proline | −Leucine MCES +Urea | Transamination to Proline using Leucine | 1 $O_2$(s) 1 Pyruvate(m) 1 Leucine(s) 1 ATP-energy(m) 3 NADPH-redox-potential(m) | 3 $H_2O$(s) 1 Proline(s) 4 NADH-redox-potential(m) 11 Proton-gradient(m) 2 CoA-activated acetyl group(m) | - | 22 | - | - | - | - | - | - | 3 | - | 7 | - |
| 241 Proline from Lysine | Proline | −Lysine MCES +Urea | Transamination to Proline using Lysine | 0.75 $O_2$(s) 1 Pyruvate(m) 0.5 Lysine(s) 1 ATP-energy(m) 2.5 NADPH-redox-potential(m) | 1.5 $H_2O$(s) 1 $CO_2$(s) 1 Proline(s) 0.5 NADH-redox-potential(c) 2.5 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 8 Proton-gradient(m) | 6 | 18 | - | - | - | - | - | - | 5 | - | 9 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 242 Proline from Methionine | Proline | −Methionine MCES +Urea +$H_2S$ | Transamination to Proline using Methionine | 0.67 $O_2$(s) 0.33 Pyruvate(m) 1 Methionine(s) 0.5 Glucose-6P(c) 1 ATP-energy(m) 2 NADPH-redox-potential(m) | 1.83 $H_2O$(s) 0.5 $P_i$(c) 1 Pyruvate(c) 1 Proline(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 16 | 25 | - | - | - | - | - | - | 6 | - | 11 | - |
| 243 Proline from Phenylalanine | Proline | −Phenylalanine MCES +Urea | Transamination to Proline using Phenylalanine | 3.5 $O_2$(s) 1 Phenylalanine(s) 2 ATP-energy(c) 1 ATP-energy(m) 1 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 2 $H_2O$(s) 2 $CO_2$(s) 1 Proline(s) 1 NADH-redox-potential(m) 6 Proton-gradient(m) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 17 | 10 | - | - | - | - | - | - | 6 | - | 7 | - |
| 244 Proline from Serine | Proline | −Serine MCES +Urea | Transamination to Proline using Serine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 Serine(s) 1 ATP-energy(m) 3 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 3 $H_2O$(s) 1 Pyruvate(c) 1 Proline(s) 2 NADH-redox-potential(m) 1 Proton-gradient(c) 5 Proton-gradient(m) 1 Na-gradient(c) | 1 | 15 | - | - | - | - | - | - | 6 | - | 7 | - |
| 245 Proline from Threonine | Proline | −Threonine MCES +Urea | Transamination to Proline using Threonine | 0.67 $O_2$(s) 0.33 Pyruvate(m) 1 Threonine(s) 1 ATP-energy(m) 2 NADPH-redox-potential(m) | 3.33 $H_2O$(s) 1 Proline(s) 1.33 NADH-redox-potential(m) 6 Proton-gradient(m) | 1 | 25 | - | - | - | - | - | - | 4 | - | 8 | - |
| 246 Proline from Tryptophan | Proline | −Tryptophan MCES +Urea | Transamination to Proline using Tryptophan | 2.25 $O_2$(s) 1 Pyruvate(m) 0.5 Tryptophan(s) 0.5 ATP-energy(c) 1 ATP-energy(m) 2.5 NADPH-redox-potential(m) | 1 $H_2O$(s) 2 $CO_2$(s) 0.5 Pyruvate(c) 1 Proline(s) 0.5 NADH-redox-potential(c) 2 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 8.5 Proton-gradient(m) 0.5 Na-gradient(c) | 17 | 16 | - | - | - | - | - | - | 7 | - | 10 | - |
| 247 Proline from Tyrosine | Proline | −Tyrosine MCES +Urea | Transamination to Proline using Tyrosine | 2.5 $O_2$(s) 1 Tyrosine(s) 2 ATP-energy(c) 1 ATP-energy(m) 1 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 1 $H_2O$(s) 2 $CO_2$(s) 1 Proline(s) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 6 Proton-gradient(m) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 15 | 11 | - | - | - | - | - | - | 6 | - | 7 | - |
| 248 Proline from Valine | Proline | −Valine MCES +Urea | Transamination to Proline using Valine | 1 $O_2$(s) 1 Valine(s) 1 ATP-energy(m) 1 NADPH-redox-potential(m) | 2 $H_2O$(s) 1 Proline(s) 2 NADH-redox-potential(m) 10 Proton-gradient(m) | - | 16 | - | - | - | - | - | - | 4 | - | 7 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 249 Proline from beta-Alanine | Proline | −beta-Alanine MCES +Urea | Transamination to Proline using beta-Alanine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 beta-Alanine(s) 1 ATP-energy(m) 2 NADPH-redox-potential(m) | 2 $H_2O$(s) 1 $CO_2$(s) 1 Proline(s) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 5 Proton-gradient(m) | 3 | 13 | - | - | - | - | - | - | 5 | - | 8 | - |
| 250 Serine from Alanine | Serine | −Alanine MCES +Urea | Transamination to Serine using Alanine | 1.5 $H_2O$(s) 1 Alanine(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 1 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 Na-gradient(c) | 12 | - | - | - | - | - | - | - | 4 | - | - | - |
| 251 Serine from Arginine | Serine | −Arginine MCES +Urea | Transamination to Serine using Arginine | 3 $H_2O$(s) 0.25 $O_2$(s) 0.5 Pyruvate(m) 0.5 Arginine(s) 0.5 Glucose-6P(c) 0.5 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 0.5 Urea(s) 0.5 ATP-energy(c) 0.5 ATP-energy(m) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1.5 Proton-gradient(m) | 14 | 11 | - | - | - | - | - | - | 7 | - | 10 | - |
| 252 Serine from Asparagine | Serine | −Asparagine MCES +Urea | Transamination to Serine using Asparagine | 1.5 $H_2O$(s) 0.5 Glucose-6P(c) 0.5 Asparagine(s) 0.5 NADPH-redox-potential(m) 1 Proton-gradient(m) | 0.5 $P_i$(c) 0.5 $CO_2$(s) 0.5 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 1.5 NADH-redox-potential(c) 0.5 NADPH-redox-potential(c) | 16 | 2 | - | - | - | - | - | - | 5 | - | 7 | - |
| 253 Serine from Aspartate | Serine | −Aspartate MCES +Urea | Transamination to Serine using Aspartate | 1.5 $H_2O$(s) 1 Aspartate(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 15 | - | - | - | - | - | - | - | 5 | - | - | - |
| 254 Serine from Cysteine | Serine | −Cysteine MCES +Urea +$H_2S$ | Transamination to Serine using Cysteine | 1.5 $H_2O$(s) 0.5 Glucose-6P(c) 1 Cysteine(s) 1 NADH-redox-potential(m) 2 Proton-gradient(m) | 0.5 $P_i$(c) 1 Pyruvate(c) 1 Serine(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 Na-gradient(c) | 12 | 2 | - | - | - | - | - | - | 5 | - | 7 | - |
| 255 Serine from Cystine | Serine | −Cystine MCES +Urea +$H_2S$ | Transamination to Serine using Cystine | 1.5 $H_2O$(s) 0.5 Glucose-6P(c) 0.5 Cystine(s) 1 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 2 Proton-gradient(m) | 0.5 $P_i$(c) 1 Pyruvate(c) 1 Serine(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 0.5 Na-gradient(c) | 14 | 2 | - | - | - | - | - | - | 6 | - | 7 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 256 Serine from Glutamate | Serine | −Glutamate MCES +Urea | Transamination to Serine using Glutamate | 2.5 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamate(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 1 ATP-energy(m) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 6 Proton-gradient(m) 1 Na-gradient(c) | 13 | 7 | - | - | - | - | - | - | 6 | - | 7 | - |
| 257 Serine from Glycine | Serine | −Glycine MCES +Urea | Transamination to Serine using Glycine | 1 $H_2O$(s) 1 Glycine(s) 1 THF-activated methyl group(c) | 1 Serine(s) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 3 | - | - | - |
| 258 Serine from Histidine | Serine | −Histidine MCES +Urea | Transamination to Serine using Histidine | 1.83 $H_2O$(s) 0.17 $O_2$(s) 0.5 Glucose-6P(c) 0.33 Histidine(s) 0.33 NADH-redox-potential(m) | 0.5 $P_i$(c) 0.67 $CO_2$(s) 0.33 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 0.33 ATP-energy(m) 1.67 NADH-redox-potential(c) 0.67 Proton-gradient(m) 0.33 THF-activated methyl group(c) | 20 | 8 | - | - | - | - | - | - | 6 | - | 12 | - |
| 259 Serine from Isoleucine | Serine | −Isoleucine MCES +Urea | Transamination to Serine using Isoleucine | 2.5 $H_2O$(s) 1 $O_2$(s) 0.5 Glucose-6P(c) 1 Isoleucine(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Serine(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 4 NADH-redox-potential(m) 9 Proton-gradient(m) 2 CoA-activated acetyl group(m) | 11 | 13 | - | - | - | - | - | - | 5 | - | 11 | - |
| 260 Serine from Glutamine | Serine | −Glutamine MCES +Urea | Transamination to Serine using Glutamine | 2 $H_2O$(s) 0.25 $O_2$(s) 0.5 Glutamine(s) 0.5 Glucose-6P(c) 0.5 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 0.5 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 0.5 ATP-energy(m) 2 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 2 Proton-gradient(m) | 15 | 9 | - | - | - | - | - | - | 5 | - | 11 | - |
| 261 Serine from Leucine | Serine | −Leucine MCES +Urea | Transamination to Serine using Leucine | 0.5 $H_2O$(s) 0.5 $O_2$(s) 0.5 Glucose-6P(c) 1 Leucine(s) 1 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 Serine(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 4 Proton-gradient(m) 1 Na-gradient(c) 3 CoA-activated acetyl group(m) | 11 | 13 | - | - | - | - | - | - | 5 | - | 10 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 262 Serine from Lysine | Serine | −Lysine MCES +Urea | Transamination to Serine using Lysine | 2 $H_2O$(s) 0.25 $O_2$(s) 0.5 Lysine(s) 0.5 Glucose-6P(c) 0.5 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Serine(s) 0.5 ATP-energy(c) 2.5 NADH-redox-potential(c) 1.5 NADH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 12 | 11 | - | - | - | - | - | - | 5 | - | 11 | - |
| 263 Serine from Methionine | Serine | −Methionine MCES +Urea +$H_2S$ | Transamination to Serine using Methionine | 3 $H_2O$(s) 0.5 $O_2$(s) 1 Methionine(s) 1 Glucose-6P(c) | 1 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 1 $H_2S$(s) 1 ATP-energy(c) 4 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 16 | 9 | - | - | - | - | - | - | 5 | - | 12 | - |
| 264 Serine from Phenylalanine | Serine | −Phenylalanine MCES +Urea | Transamination to Serine using Phenylalanine | 1.5 $H_2O$(s) 3 $O_2$(s) 1 Phenylalanine(s) 0.5 Glucose-6P(c) 1.5 ATP-energy(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 2 NADH-redox-potential(c) 2 CoA-activated acetyl group(c) | 25 | - | - | - | - | - | - | - | 5 | - | - | - |
| 265 Serine from Proline | Serine | −Proline MCES +Urea | Transamination to Serine using Proline | 5.5 $H_2O$(s) 0.5 Glucose-6P(c) 1 Proline(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 1 ATP-energy(m) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 13 | 10 | - | - | - | - | - | - | 5 | - | 4 | - |
| 266 Serine from Threonine | Serine | −Threonine MCES +Urea | Transamination to Serine using Threonine | 1.5 $H_2O$(s) 0.5 $O_2$(s) 0.5 Glucose-6P(c) 1 Threonine(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Serine(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 12 | 9 | - | - | - | - | - | - | 5 | - | 11 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 267 Serine from Tryptophan | Serine | −Tryptophan MCES +Urea | Transamination to Serine using Tryptophan | 1.5 $H_2O$(s) 1.75 $O_2$(s) 0.5 Tryptophan(s) 0.5 Glucose-6P(c) 1.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1.5 $CO_2$(s) 0.5 Pyruvate(c) 1 Serine(s) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1.5 Proton-gradient(m) 0.5 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 25 | 9 | - | - | - | - | - | - | 6 | - | 12 | - |
| 268 Serine from Tyrosine | Serine | −Tyrosine MCES +Urea | Transamination to Serine using Tyrosine | 2.5 $H_2O$(s) 2 $O_2$(s) 1 Tyrosine(s) 0.5 Glucose-6P(c) 1.5 ATP-energy(c) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 2 NADH-redox-potential(c) 1 NADPH-redox-potential(c) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 24 | - | - | - | - | - | - | - | 6 | - | - | - |
| 269 Serine from Valine | Serine | −Valine MCES +Urea | Transamination to Serine using Valine | 3.5 $H_2O$(s) 1 $O_2$(s) 0.5 Glucose-6P(c) 1 Valine(s) | 0.5 $P_i$(c) 2 $CO_2$(s) 1 Pyruvate(c) 1 Serine(s) 0.5 ATP-energy(c) 1 ATP-energy(m) 2 NADH-redox-potential(c) 3 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 10 Proton-gradient(m) 1 Na-gradient(c) | 13 | 14 | - | - | - | - | - | - | 6 | - | 10 | - |
| 270 Serine from beta-Alanine | Serine | −beta-Alanine MCES +Urea | Transamination to Serine using beta-Alanine | 1.5 $H_2O$(s) 0.5 Glucose-6P(c) 1 beta-Alanine(s) 2 Proton-gradient(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 1 Serine(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 11 | 4 | - | - | - | - | - | - | 4 | - | 7 | - |
| 271 Tyrosine from Phenylalanine | Tyrosine | −Phenylalanine MCES +Urea | Transamination to Tyrosine using Phenylalanine | 1 $O_2$(s) 1 Phenylalanine(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 Tyrosine(s) | 3 | - | - | - | - | - | - | - | 3 | - | - | - |
| 272 beta-Alanine from Alanine | beta-Alanine | −Alanine MCES +Urea | Transamination to beta-Alanine using Alanine | 1 Alanine(s) 1 NADPH-redox-potential(c) | 1 beta-Alanine(s) 1 NADH-redox-potential(c) | 7 | - | - | - | - | - | - | - | 2 | - | - | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 273 beta-Alanine from Arginine | beta-Alanine | −Arginine MCES +Urea | Transamination to beta-Alanine using Arginine | 1.5 $H_2O$(s) 0.25 $O_2$(s) 0.5 Pyruvate(m) 0.5 Arginine(s) 0.5 NADPH-redox-potential(m) | 1 $CO_2$(s) 0.5 Urea(s) 1 beta-Alanine(s) 0.5 ATP-energy(m) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1.5 Proton-gradient(m) | 5 | 11 | - | - | - | - | - | - | 6 | - | 10 | - |
| 274 beta-Alanine from Asparagine | beta-Alanine | −Asparagine MCES +Urea | Transamination to beta-Alanine using Asparagine | 0.5 Pyruvate(c) 0.5 Asparagine(s) 0.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) 1 Proton-gradient(m) | 0.5 $CO_2$(s) 1 beta-Alanine(s) 0.5 NADH-redox-potential(c) | 7 | 2 | - | - | - | - | - | - | 3 | - | 7 | - |
| 275 beta-Alanine from Aspartate | beta-Alanine | −Aspartate MCES +Urea | Transamination to beta-Alanine using Aspartate | 1 Aspartate(s) | 1 $CO_2$(s) 1 beta-Alanine(s) 1 Na-gradient(c) | 1 | - | - | - | - | - | - | - | 4 | - | - | - |
| 276 beta-Alanine from Cysteine | beta-Alanine | −Cysteine MCES +Urea +$H_2S$ | Transamination to beta-Alanine using Cysteine | 1 Pyruvate(m) 1 Cysteine(s) 2 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 Pyruvate(c) 1 beta-Alanine(s) 1 $H_2S$(s) 1 NADH-redox-potential(c) | 5 | 3 | - | - | - | - | - | - | 3 | - | 7 | - |
| 277 beta-Alanine from Cystine | beta-Alanine | −Cystine MCES +Urea +$H_2S$ | Transamination to beta-Alanine using Cystine | 0.5 Cystine(s) 1.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 1 beta-Alanine(s) 1 $H_2S$(s) 1 NADH-redox-potential(c) 0.5 Na-gradient(c) | 8 | 2 | - | - | - | - | - | - | 5 | - | 7 | - |
| 278 beta-Alanine from Glutamate | beta-Alanine | −Glutamate MCES +Urea | Transamination to beta-Alanine using Glutamate | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamate(s) | 2 $CO_2$(s) 1 beta-Alanine(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 6 Proton-gradient(m) 1 Na-gradient(c) | 4 | 7 | - | - | - | - | - | - | 6 | - | 7 | - |
| 279 beta-Alanine from Glycine | beta-Alanine | −Glycine MCES +Urea | Transamination to beta-Alanine using Glycine | 1 Glycine(s) 1 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 1 beta-Alanine(s) 1 NADH-redox-potential(c) 1 Na-gradient(c) | 16 | - | - | - | - | - | - | - | 3 | - | - | - |
| 280 beta-Alanine from Histidine | beta-Alanine | −Histidine MCES +Urea | Transamination to beta-Alanine using Histidine | 0.33 $H_2O$(s) 0.17 $O_2$(s) 0.67 Pyruvate(m) 0.33 Histidine(s) 0.67 NADPH-redox-potential(c) 1.33 NADPH-redox-potential(m) | 0.67 $CO_2$(s) 1 beta-Alanine(s) 0.67 NADH-redox-potential(c) 0.67 NADH-redox-potential(m) 1.67 Proton-gradient(m) 0.33 Na-gradient(c) 0.33 THF-activated methyl group(c) | 13 | 13 | - | - | - | - | - | - | 6 | - | 10 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 281 beta-Alanine from Isoleucine | beta-Alanine | −Isoleucine MCES +Urea | Transamination to beta-Alanine using Isoleucine | 1 $H_2O$(s) 1 $O_2$(s) 1 Isoleucine(s) | 1 $CO_2$(s) 1 beta-Alanine(s) 3 NADH-redox-potential(m) 11 Proton-gradient(m) 1 CoA-activated acetyl group(m) | - | 13 | - | - | - | - | - | - | 5 | - | 8 | - |
| 282 beta-Alanine from Glutamine | beta-Alanine | −Glutamine MCES +Urea | Transamination to beta-Alanine using Glutamine | 0.5 $H_2O$(s) 0.25 $O_2$(s) 0.5 Pyruvate(m) 0.5 Glutamine(s) 0.5 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 beta-Alanine(s) 0.5 ATP-energy(m) 1 NADH-redox-potential(c) 0.5 Proton-gradient(c) 2.5 Proton-gradient(m) 0.5 Na-gradient(c) | 6 | 9 | - | - | - | - | - | - | 7 | - | 8 | - |
| 283 beta-Alanine from Leucine | beta-Alanine | −Leucine MCES +Urea | Transamination to beta-Alanine using Leucine | 0.5 $O_2$(s) 1 Pyruvate(m) 1 Leucine(s) 2 NADPH-redox-potential(m) | 1 $H_2O$(s) 1 beta-Alanine(s) 3 NADH-redox-potential(m) 3 Proton-gradient(m) 1 Na-gradient(c) 3 CoA-activated acetyl group(m) | 1 | 14 | - | - | - | - | - | - | 5 | - | 10 | - |
| 284 beta-Alanine from Lysine | beta-Alanine | −Lysine MCES +Urea | Transamination to beta-Alanine using Lysine | 0.5 $H_2O$(s) 0.25 $O_2$(s) 1 Pyruvate(m) 0.5 Lysine(s) 1.5 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 beta-Alanine(s) 0.5 NADH-redox-potential(c) 2.5 NADH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 3 | 14 | - | - | - | - | - | - | 5 | - | 9 | - |
| 285 beta-Alanine from Methionine | beta-Alanine | −Methionine MCES +Urea +$H_2S$ | Transamination to beta-Alanine using Methionine | 1.5 $H_2O$(s) 0.5 $O_2$(s) 1 Pyruvate(m) 1 Methionine(s) 0.5 Glucose-6P(c) 1 NADPH-redox-potential(m) | 0.5 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 1 beta-Alanine(s) 1 $H_2S$(s) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) 1 NADPH-redox-potential(c) 4 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 18 | 9 | - | - | - | - | - | - | 7 | - | 11 | - |
| 286 beta-Alanine from Phenylalanine | beta-Alanine | −Phenylalanine MCES +Urea | Transamination to beta-Alanine using Phenylalanine | 3 $O_2$(s) 1 Phenylalanine(s) 2 ATP-energy(c) | 2 $CO_2$(s) 1 beta-Alanine(s) 2 CoA-activated acetyl group(c) | 17 | - | - | - | - | - | - | - | 4 | - | - | - |
| 287 beta-Alanine from Proline | beta-Alanine | −Proline MCES +Urea | Transamination to beta-Alanine using Proline | 4 $H_2O$(s) 1 Proline(s) | 2 $CO_2$(s) 1 beta-Alanine(s) 1 ATP-energy(m) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 1 Na-gradient(c) | 4 | 10 | - | - | - | - | - | - | 5 | - | 4 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 288 beta-Alanine from Serine | beta-Alanine | −Serine MCES +Urea | Transamination to beta-Alanine using Serine | 1 Serine(s) 2 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 beta-Alanine(s) 1 NADH-redox-potential(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 13 | - | - | - | - | - | - | - | 5 | - | - | - |
| 289 beta-Alanine from Threonine | beta-Alanine | −Threonine MCES +Urea | Transamination to beta-Alanine using Threonine | 0.5 $O_2$(s) 1 Threonine(s) | 1 $CO_2$(s) 1 beta-Alanine(s) 1 NADH-redox-potential(m) 5 Proton-gradient(m) | 1 | 8 | - | - | - | - | - | - | 4 | - | 8 | - |
| 290 beta-Alanine from Tryptophan | beta-Alanine | −Tryptophan MCES +Urea | Transamination to beta-Alanine using Tryptophan | 1.75 $O_2$(s) 1 Pyruvate(m) 0.5 Tryptophan(s) 0.5 ATP-energy(c) 2 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 1.5 $CO_2$(s) 0.5 Pyruvate(c) 1 beta-Alanine(s) 1.5 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 2.5 Proton-gradient(m) 0.5 Na-gradient(c) 0.5 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 20 | 10 | - | - | - | - | - | - | 5 | - | 10 | - |
| 291 beta-Alanine from Tyrosine | beta-Alanine | −Tyrosine MCES +Urea | Transamination to beta-Alanine using Tyrosine | 1 $H_2O$(s) 2 $O_2$(s) 1 Tyrosine(s) 2 ATP-energy(c) | 2 $CO_2$(s) 1 beta-Alanine(s) 1 NADH-redox-potential(c) 1 Na-gradient(c) 2 CoA-activated acetyl group(c) | 16 | - | - | - | - | - | - | - | 6 | - | - | - |
| 292 beta-Alanine from Valine | beta-Alanine | −Valine MCES +Urea | Transamination to beta-Alanine using Valine | 2 $H_2O$(s) 1 $O_2$(s) 1 Valine(s) | 2 $CO_2$(s) 1 beta-Alanine(s) 4 NADH-redox-potential(m) 11 Proton-gradient(m) | - | 13 | - | - | - | - | - | - | 5 | - | 8 | - |
| 293 Homocysteine from Methionine | Homocysteine(c) | −Methionine(c) MCES | test that cytosolic Homocysteine can be produced from Methionine | 1 Methionine(c) | 1 Homocysteine(c) 1 THF-activated methyl group(c) | 2 | - | - | - | - | - | - | - | - | - | - | - |
| 294 Taurine from Methionine | Taurine | −Methionine MCES | Conversion of methionine in taurine | 2.5 $H_2O$(s) 1.5 $O_2$(s) 1 Methionine(s) 0.5 Glucose-6P(c) | 0.5 $P_i$(c) 3 $CO_2$(s) 1 Taurine(s) 0.5 ATP-energy(c) 3 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 18 | 9 | - | - | - | - | - | - | 6 | - | 11 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 295 Taurine from Cysteine | Taurine | −Cysteine MCES | Conversion of methionine in taurine | 1 $H_2O$(s) 1 $O_2$(s) 1 Cysteine(s) | 1 $CO_2$(s) 1 Taurine(s) 1 NADH-redox-potential(c) | 4 | - | - | - | - | - | - | - | 5 | - | - | - |
| **B2.3. Fatty acid conversion** **B2.3.1. Saturated** | | | | | | | | | | | | | | | | | |
| 296 Stearate from Palmitate | Stearate | −Palmitate MCES | Conversion of Palmitate into Stearate | 1 Palmitate(s) 3 ATP-energy(c) 1 NADH-redox-potential(m) 1 FADH-redox-potential(c) 1 CoA-activated acetyl group(m) | 1 $H_2O$(s) 1 Stearate(s) | 8 | 6 | - | - | - | - | - | - | 3 | - | 4 | - |
| **B2.3.2. Omega-3-Fatty acids** | | | | | | | | | | | | | | | | | |
| 297 Palmitate from Palmitolate | Palmitate | −Palmitolate MCES | Conversion of Palmitolate into Palmitate | 1 Palmitolate(s) 4 ATP-energy(c) 2 NADPH-redox-potential(c) | 1 Palmitate(s) 1 NADH-redox-potential(c) | 17 | - | - | - | - | - | - | - | 2 | - | - | - |
| 298 Palmitolate from Palmitate | Palmitolate | −Palmitate MCES | Conversion of Palmitate into Palmitolate | 1 $O_2$(s) 1 Palmitate(s) 1 ATP-energy(c) 1 NADH-redox-potential(c) | 2 $H_2O$(s) 1 Palmitolate(s) | 6 | - | - | - | - | - | - | - | 4 | - | - | - |
| 299 Oleate from Stearate | Oleate | −Stearate MCES | Conversion of Stearate into Oleate | 1 $O_2$(s) 1 Stearate(s) 3 ATP-energy(c) 1 NADH-redox-potential(c) | 2 $H_2O$(s) 1 Oleate(s) | 7 | - | - | - | - | - | - | - | 4 | - | - | - |
| 300 Stearate from Oleate | Stearate | −Oleate MCES | Conversion of into Stearate | 1 Oleate(s) 4 ATP-energy(c) 2 NADPH-redox-potential(c) | 1 Stearate(s) 1 NADH-redox-potential(c) | 16 | - | - | - | - | - | - | - | 2 | - | - | - |
| 301 Palmitolate from Arachidonate | Palmitolate | −Arachidonate MCES | Conversion of from Arachidonate | 1 $O_2$(s) 8 ATP-energy(c) 1 NADH-redox-potential(c) 14 NADPH-redox-potential(c) 8 CoA-activated acetyl group(c) | 8 $H_2O$(s) 1 Palmitolate(s) | 42 | - | - | - | - | - | - | - | 3 | - | - | - |
| **B2.3.3. Omega-6-Fatty acids** | | | | | | | | | | | | | | | | | |
| 302 gamma-Linolenate from Linoleate | gamma-Linolenate | −Linoleate MCES | Conversion of Linoleate into gamma-Linolenate | 1 $O_2$(s) 1 Linoleate(s) 3 ATP-energy(c) 1 NADH-redox-potential(c) | 1 $H_2O$(s) 1 gamma-Linolenate(s) | 7 | - | - | - | - | - | - | - | 4 | - | - | - |
| 303 Dihomo-gamma-linolenate from Linoleate | Dihomo-gamma-linolenate | −Linoleate MCES | Conversion of Linoleate into Dihomo-gamma-linolenate | 2 $O_2$(s) 1 Linoleate(s) 4 ATP-energy(c) 1 NADH-redox-potential(c) 4 NADPH-redox-potential(r) 1 CoA-activated acetyl group(c) | 4 $H_2O$(s) 1 Dihomo-gamma-linolenate(s) | 12 | - | 3 | - | - | - | - | - | 4 | - | 6 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 304 Arachidonate from Linoleate | Arachidonate | −Linoleate MCES | Conversion of Linoleate into Arachidonate | 3 $O_2$(s) 1 Linoleate(s) 4 ATP-energy(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(r) 1 CoA-activated acetyl group(c) | 5 $H_2O$(s) 1 Arachidonate(s) | 13 | - | 3 | - | - | - | - | - | 4 | - | 6 | - |
| 305 Dihomo-gamma-linolenate from gamma-Linolenate | Dihomo-gamma-linolenate | −gamma-Linolenate MCES | Conversion of gamma-Linolenate into Dihomo-gamma-linolenate | 1 $O_2$(s) 1 gamma-Linolenate(s) 4 ATP-energy(c) 4 NADPH-redox-potential(r) 1 CoA-activated acetyl group(c) | 3 $H_2O$(s) 1 Dihomo-gamma-linolenate(s) | 10 | - | 3 | - | - | - | - | - | 4 | - | 6 | - |
| 306 Arachidonate from gamma-Linolenate | Arachidonate | −gamma-Linolenate MCES | Conversion of gamma-Linolenate into Arachidonate | 2 $O_2$(s) 1 gamma-Linolenate(s) 4 ATP-energy(c) 1 NADH-redox-potential(c) 4 NADPH-redox-potential(r) 1 CoA-activated acetyl group(c) | 4 $H_2O$(s) 1 Arachidonate(s) | 12 | - | 3 | - | - | - | - | - | 4 | - | 6 | - |
| 307 Arachidonate from Dihomo-gamma-linolenate | Arachidonate | −Dihomo-gamma-linolenate MCES | Conversion of Dihomo-gamma-linolenate into Arachidonate | 1 $O_2$(s) 1 Dihomo-gamma-linolenate(s) 3 ATP-energy(c) 1 NADH-redox-potential(c) | 1 $H_2O$(s) 1 Arachidonate(s) | 7 | - | - | - | - | - | - | - | 4 | - | - | - |
| **B2.4. Lipoproteins** | | | | | | | | | | | | | | | | | |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 308 VLDL from LDL | VLDL | −LDL MCES =Cysteine +Methionine =Leucine =Isoleucine =Histidine =Asparagine =Valine =Tryptophan =Lysine =Phenylalanine =Threonine =Tyrosine =Valine =Ethanolamine(c) =Choline(c) ALFA | Lipoprotein conversion VLDL from LDL | 381.4 Pyruvate(m) 99.1 Lysine(s) 56.8 Tryptophan(s) 33.1 Phenylalanine(s) 31.4 Tyrosine(s) 6074 Glucose-6P(c) 695.2 Cysteine(s) 2489 Choline(c) 299.1 Leucine(s) 16.6 Histidine(s) 917.6 Asparagine(s) 173.7 Valine(s) 771.4 Threonine(s) 311.4 Ethanolamine(c) 1277 Arachidonate(c) 11891 Palmitate(c) 20.5 Isoleucine(s) 12595 Oleate(c) 2193 Stearate(c) 8299 Linoleate(c) 0.98 LDL(s) $1.2{\cdot}10^5$ ATP-energy(c) 784.1 ATP-energy(m) 12485 NADH-redox-potential(c) 508.6 NADPH-redox-potential(c) 1332 NADPH-redox-potential(m) 649.3 Proton-gradient(m) 549.9 THF-activated methyl group(c) 709.8 CoA-activated acetyl group(m) | 34610 $H_2O$(s) 3643 $P_i$(c) 1239 $CO_2$(s) 107.5 Pyruvate(c) 622.8 Methionine(s) 1 VLDL(s) 1440 NADH-redox-potential(m) 450.8 Proton-gradient(c) 1318 Na-gradient(c) | 94 | 21 | 17 | - | - | - | - | - | 18 | - | 63 | 5 |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 309 VLDL from HDL | VLDL | −HDL MCES =Cysteine +Methionine =Leucine =Isoleucine =Histidine =Asparagine =Valine =Tryptophan =Lysine =Phenylalanine =Threonine =Tyrosine =Valine =Ethanolamine(c) =Choline(c) ALFA | Lipoprotein conversion VLDL from HDL | 49 Pyruvate(m) 73.8 Phenylalanine(s) 23.1 Tyrosine(s) 5626 Glucose-6P(c) 84.9 Cysteine(s) 1247 Choline(c) 47.3 Asparagine(s) 85.9 Valine(s) 116.7 Threonine(s) 4817 Arachidonate(c) 10414 Palmitate(c) 299 Isoleucine(s) 3845 Farnesyl-PP(r) 14488 Oleate(c) 3419 Linoleate(c) 1344 gamma-Linolenate(c) 11.1 HDL(s) $1.2{\cdot}10^5$ ATP-energy(c) 18.7 ATP-energy(m) 35.3 NADH-redox-potential(m) 5767 NADPH-redox-potential(r) 49 NADPH-redox-potential(m) 67.6 Proton-gradient(m) | 18479 $H_2O$(s) 12494 $P_i$(c) 5674 $CO_2$(s) 167.4 Pyruvate(c) 42 Lysine(s) 18.4 Tryptophan(s) 93.3 Leucine(s) 4.65 Histidine(s) 93.4 Ethanolamine(c) 205.6 Stearate(c) 1 VLDL(s) 1922 NADH-redox-potential(r) 194 NADH-redox-potential(c) 1959 NADPH-redox-potential(c) 47.3 Proton-gradient(c) 627.3 Na-gradient(c) 42.1 THF-activated methyl group(c) 3845 CoA-activated acetyl group(c) | 83 | 16 | 33 | - | - | - | - | - | 17 | - | 64 | 5 |
| **B2.5. Bilirubin** | | | | | | | | | | | | | | | | | |
| 310 Bilirubin conjugation | Bilirubin-bisglucuronoside(b) | MCES −Bilirubin | Bilirubin import, conjugation, and export | 2 $H_2O$(s) 2 Glucose-6P(c) 1 Bilirubin(s) 5 ATP-energy(c) | 2 $P_i$(c) 1 Bilirubin-bisglucuronoside(b) 4 NADH-redox-potential(c) | 8 | - | 2 | - | - | - | - | - | 2 | 1 | 5 | - |
| **B2.6. Urea** | | | | | | | | | | | | | | | | | |
| 311 Urea from glutamine | Urea | MCES −Glutamine | Urea from glutamine | 2 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamine(s) 2 ATP-energy(c) 1 ATP-energy(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Urea(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Proton-gradient(c) 6 Proton-gradient(m) 1 Na-gradient(c) | 14 | 9 | - | - | - | - | - | - | 7 | - | 7 | - |
| 312 Urea from alanine | Urea | MCES −Alanine | Urea from alanine | 1 $H_2O$(s) 2 Alanine(s) 2 ATP-energy(c) 2 ATP-energy(m) | 1 Pyruvate(c) 1 Urea(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 11 | 9 | - | - | - | - | - | - | 3 | - | 2 | - |

Continued on next page

B2. Turnover functions – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 313 Urea from $NH_3$ | Urea | MCES $-NH_3$ | Urea from alanine | 1 $H_2O$(s) 2 Alanine(s) 2 ATP-energy(c) 2 ATP-energy(m) | 1 Pyruvate(c) 1 Urea(s) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 11 | 9 | - | - | - | - | - | - | 3 | - | 2 | - |
| **B2.7. Creatine** | | | | | | | | | | | | | | | | | |
| 314 Creatine | Creatine(c) | MCES $-$Arginine $-$Glycine | de novo synthesis of cytosolic Creatine | 1 $H_2O$(s) 0.25 $O_2$(s) 1 Glycine(s) 0.5 Arginine(s) 1 Activated methyl group(c) 1 ATP-energy(c) 0.5 ATP-energy(m) | 0.5 $CO_2$(s) 0.5 Pyruvate(c) 1 Creatine(c) 2 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 1.5 Proton-gradient(m) | 11 | 14 | - | - | - | - | - | - | 5 | - | 11 | - |

## 3.3 B3. Excretion of de novo synthesized substances

Table 10: B3. Excretion of de novo synthesized substances



| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| **B3.1. Bile excretion** | | | | | | | | | | | | | | | | | |
| **B3.1.1. Bile acids** | | | | | | | | | | | | | | | | | |
| 315 Glycocholate(b) | Glycocholate(b) | +Urea $-$Alanine $-$Serine MCES | de novo synthesis and bile export of Glycocholate | 12 $O_2$(s) 1 Serine(s) 2 Farnesyl-PP(r) 5 ATP-energy(c) 12 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) 1 Proton-gradient(c) | 10 $H_2O$(s) 4 $P_i$(c) 4 $CO_2$(s) 1 Glycocholate(b) 1 NADH-redox-potential(r) 2 NADH-redox-potential(m) 1 NADH-redox-potential(p) 6 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 15 | 7 | 19 | 7 | - | - | - | - | 5 | 1 | 21 | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 316 Gly-CD-cholate(b) | Glycochenodeoxycholate(b) | +Urea −Alanine −Serine MCES | de novo synthesis and bile export of Glycochenodeoxycholate from Palmitate, Alanine, Serine, excreting urea and $CO_2$ | 10.5 $O_2$(s) 1 Serine(s) 2 Farnesyl-PP(r) 5 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(m) 1 Proton-gradient(c) | 8 $H_2O$(s) 4 $P_i$(c) 4 $CO_2$(s) 1 Glycochenodeoxycholate(b) 1 NADH-redox-potential(r) 2 NADH-redox-potential(m) 6 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 13 | 9 | 18 | 2 | - | - | - | - | 5 | 1 | 22 | - | |
| 317 Taurocholate(b) | Taurocholate(b) | +Urea −Alanine −Serine −Methionine MCES | de novo synthesis and bile export of Taurocholate | 13.5 $O_2$(s) 1 Serine(s) 1 Methionine(s) 2 Farnesyl-PP(r) 6 ATP-energy(c) 1 ATP-energy(m) 12 NADPH-redox-potential(r) 2 NADPH-redox-potential(c) | 7.5 $H_2O$(s) 4 $P_i$(c) 6.5 $CO_2$(s) 0.5 Urea(s) 1 Taurocholate(b) 1 NADH-redox-potential(r) 3.5 NADH-redox-potential(c) 4.5 NADH-redox-potential(m) 1 NADH-redox-potential(p) 1 Proton-gradient(c) 10 Proton-gradient(m) 2 Na-gradient(c) 1 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 26 | 12 | 19 | 7 | - | - | - | - | 8 | 1 | 28 | - | |
| 318 tcdchola(b) | Taurochenodeoxycholate(b) | +Urea −Alanine −Serine −Methionine MCES | de novo synthesis and bile export of Taurochenodeoxycholate | 12 $O_2$(s) 1 Serine(s) 1 Methionine(s) 2 Farnesyl-PP(r) 7 ATP-energy(c) 1 ATP-energy(m) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 5.5 $H_2O$(s) 4 $P_i$(c) 6.5 $CO_2$(s) 0.5 Urea(s) 1 Taurochenodeoxycholate(b) 1 NADH-redox-potential(r) 3.5 NADH-redox-potential(c) 4.5 NADH-redox-potential(m) 10 Proton-gradient(m) 1 Na-gradient(c) 1 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 25 | 14 | 18 | 2 | - | - | - | - | 7 | 1 | 29 | - | |
| 319 Chenodiol(b) | Chenodiol(b) | +Urea −Alanine −Serine MCES | de novo synthesis and bile export of Chenodiol | 10.5 $O_2$(s) 2 Farnesyl-PP(r) 4 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(m) | 6 $H_2O$(s) 4 $P_i$(c) 4 $CO_2$(s) 1 Chenodiol(b) 1 NADH-redox-potential(r) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 6 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 10 | 9 | 18 | 2 | - | - | - | - | 3 | 1 | 22 | - | |
| **B3.1.2. Phospholipids** | | | | | | | | | | | | | | | | | | |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 320 Bile-PC(b) | Bile-PC-pool(b) | MCES ALFA | de novo synthesis and bile export of Bile-PC-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Choline(c) 0.11 Arachidonate(c) 0.83 Palmitate(c) 0.24 Oleate(c) 0.11 Stearate(c) 0.66 Linoleate(c) 0.05 Palmitolate(c) 8.5 ATP-energy(c) 1 NADH-redox-potential(c) | 3.5 $H_2O$(s) 1 Bile-PC-pool(b) | 30 | - | - | - | - | - | - | - | 1 | 1 | - | - | |
| 321 SM(b) | SM-pool(b) | MCES ALFA | de novo synthesis and bile export of SM-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Choline(c) 1 Ethanolamine(c) 0.02 Arachidonate(c) 0.91 Palmitate(c) 0.24 Oleate(c) 0.03 gamma-Linolenate(c) 0.8 Palmitolate(c) 10.5 ATP-energy(c) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 3.53 $H_2O$(s) 1 $CO_2$(s) 1 SM-pool(b) 3 NADH-redox-potential(c) 1 CoA-activated acetyl group(c) | 37 | 2 | 1 | - | - | - | - | - | 2 | 1 | 11 | - | |
| 322 PS(b) | PS-VLDL-pool(b) | MCES ALFA | de novo synthesis and bile export of PS-VLDL-pool | 0.5 $P_i$(c) 1 Pyruvate(m) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 0.53 Arachidonate(c) 0.09 Palmitate(c) 0.09 Oleate(c) 1.25 Stearate(c) 0.05 Linoleate(c) 7.5 ATP-energy(c) 1 NADH-redox-potential(c) | 3.5 $H_2O$(s) 1 PS-VLDL-pool(b) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 29 | 3 | - | - | - | - | - | - | 1 | 1 | 1 | - | |
| 323 PE(b) | PE-VLDL-pool(b) | MCES ALFA | de novo synthesis and bile export of PE-VLDL-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 0.6 Arachidonate(c) 0.34 Palmitate(c) 0.17 Oleate(c) 0.54 Stearate(c) 0.36 Linoleate(c) 8.5 ATP-energy(c) 1 NADH-redox-potential(c) | 3.5 $H_2O$(s) 1 PE-VLDL-pool(b) | 28 | - | - | - | - | - | - | - | 1 | 1 | - | - | |
| **B3.1.3. Cholesterol** | | | | | | | | | | | | | | | | | | |
| 324 Cholesterol(b) | Cholesterol(b) | MCES | de novo synthesis and bile export of Cholesterol | 8 $O_2$(s) 2 Farnesyl-PP(r) 3 ATP-energy(c) 10 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol(b) 1 NADPH-redox-potential(c) | 5 | - | 15 | - | - | - | - | - | 3 | 1 | 7 | - | |
| **B3.2. blood excretion** | | | | | | | | | | | | | | | | | | |
| **B3.2.1. Plasma proteins** | | | | | | | | | | | | | | | | | | |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 325 Albumin | Albumin | MCES AAA | de novo synthesis and export of Albumin | 62 Glutamate(s) 13 Glycine(s) 63 Alanine(s) 60 Lysine(s) 36 Aspartate(s) 27 Arginine(s) 20 Glutamine(s) 28 Serine(s) 7 Methionine(s) 2 Tryptophan(s) 35 Phenylalanine(s) 19 Tyrosine(s) 35 Cysteine(s) 64 Leucine(s) 16 Histidine(s) 24 Proline(s) 17 Asparagine(s) 43 Valine(s) 29 Threonine(s) 9 Isoleucine(s) 3045 ATP-energy(c) 46 Proton-gradient(c) | 1 Albumin(s) 239 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |
| 326 Fibrinogen | Fibrinogen | MCES AAA | de novo synthesis and export of Fibrinogen | 186 Glutamate(s) 262 Glycine(s) 134 Alanine(s) 154 Lysine(s) 176 Aspartate(s) 134 Arginine(s) 110 Glutamine(s) 278 Serine(s) 48 Methionine(s) 60 Tryptophan(s) 98 Phenylalanine(s) 98 Tyrosine(s) 48 Cysteine(s) 166 Leucine(s) 62 Histidine(s) 114 Proline(s) 138 Asparagine(s) 122 Valine(s) 182 Threonine(s) 104 Isoleucine(s) 13370 ATP-energy(c) | 1 Fibrinogen(s) 4 Proton-gradient(c) 1044 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |
| 327 Antichymotrypsin | Antichymotrypsin | MCES AAA | de novo synthesis and export of Antichymotrypsin | 29 Glutamate(s) 16 Glycine(s) 34 Alanine(s) 26 Lysine(s) 25 Aspartate(s) 16 Arginine(s) 17 Glutamine(s) 30 Serine(s) 14 Methionine(s) 3 Tryptophan(s) 25 Phenylalanine(s) 9 Tyrosine(s) 3 Cysteine(s) 59 Leucine(s) 9 Histidine(s) 16 Proline(s) 19 Asparagine(s) 24 Valine(s) 29 Threonine(s) 20 Isoleucine(s) 2115 ATP-energy(c) 15 Proton-gradient(c) | 1 Antichymotrypsin(s) 163 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 328 Antitrypsin | Antitrypsin | MCES AAA | de novo synthesis and export of Antitrypsin | 32 Glutamate(s) 24 Glycine(s) 26 Alanine(s) 34 Lysine(s) 24 Aspartate(s) 7 Arginine(s) 18 Glutamine(s) 25 Serine(s) 10 Methionine(s) 3 Tryptophan(s) 27 Phenylalanine(s) 6 Tyrosine(s) 3 Cysteine(s) 51 Leucine(s) 13 Histidine(s) 19 Proline(s) 19 Asparagine(s) 27 Valine(s) 30 Threonine(s) 20 Isoleucine(s) 2090 ATP-energy(c) 7 Proton-gradient(c) | 1 Antitrypsin(s) 171 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |
| 329 ApoA1 | ApoA1 | MCES AAA | de novo synthesis and export of ApoA1 | 30 Glutamate(s) 11 Glycine(s) 23 Alanine(s) 22 Lysine(s) 16 Aspartate(s) 17 Arginine(s) 19 Glutamine(s) 16 Serine(s) 4 Methionine(s) 5 Tryptophan(s) 8 Phenylalanine(s) 7 Tyrosine(s) 41 Leucine(s) 6 Histidine(s) 10 Proline(s) 5 Asparagine(s) 15 Valine(s) 12 Threonine(s) 1335 ATP-energy(c) | 1 ApoA1(s) 8 Proton-gradient(c) 122 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 330 ApoB100(r) | ApoB100(r) | MCES AAA | de novo synthesis of ApoB100 in ER/Golgi | 298 Glutamate(s) 207 Glycine(s) 275 Alanine(s) 357 Lysine(s) 233 Aspartate(s) 150 Arginine(s) 230 Glutamine(s) 392 Serine(s) 79 Methionine(s) 37 Tryptophan(s) 224 Phenylalanine(s) 151 Tyrosine(s) 25 Cysteine(s) 533 Leucine(s) 115 Histidine(s) 171 Proline(s) 247 Asparagine(s) 252 Valine(s) 300 Threonine(s) 285 Isoleucine(s) 22805 ATP-energy(c) | 1 ApoB100(r) 40 Proton-gradient(c) 2259 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 22 | - | 1 | 1 |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 331 ApoC1(c) | ApoC1(c) | MCES AAA | de novo synthesis of cytosolic ApoC1 | 8 Glutamate(s) 3 Glycine(s) 5 Alanine(s) 9 Lysine(s) 4 Aspartate(s) 4 Arginine(s) 3 Glutamine(s) 9 Serine(s) 2 Methionine(s) 1 Tryptophan(s) 4 Phenylalanine(s) 12 Leucine(s) 4 Proline(s) 1 Asparagine(s) 7 Valine(s) 3 Threonine(s) 4 Isoleucine(s) 415 ATP-energy(c) 2 Proton-gradient(c) | 1 ApoC1(c) 38 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 19 | - | - | 1 |
| 332 ApoC2(c) | ApoC2(c) | MCES AAA | de novo synthesis of cytosolic ApoC2 | 8 Glutamate(s) 5 Glycine(s) 7 Alanine(s) 6 Lysine(s) 4 Aspartate(s) 2 Arginine(s) 8 Glutamine(s) 9 Serine(s) 3 Methionine(s) 1 Tryptophan(s) 4 Phenylalanine(s) 5 Tyrosine(s) 15 Leucine(s) 5 Proline(s) 1 Asparagine(s) 7 Valine(s) 10 Threonine(s) 1 Isoleucine(s) 505 ATP-energy(c) 4 Proton-gradient(c) | 1 ApoC2(c) 40 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 20 | - | - | 1 |
| 333 ApoC3(c) | ApoC3(c) | MCES AAA | de novo synthesis of cytosolic ApoC3 | 5 Glutamate(s) 3 Glycine(s) 15 Alanine(s) 6 Lysine(s) 7 Aspartate(s) 4 Arginine(s) 6 Glutamine(s) 12 Serine(s) 3 Methionine(s) 3 Tryptophan(s) 4 Phenylalanine(s) 2 Tyrosine(s) 11 Leucine(s) 1 Histidine(s) 3 Proline(s) 9 Valine(s) 5 Threonine(s) 495 ATP-energy(c) 3 Proton-gradient(c) | 1 ApoC3(c) 43 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 19 | - | - | 1 |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 334 ApoE(c) | ApoE(c) | MCES AAA | de novo synthesis of cytosolic ApoE | 40 Glutamate(s) 18 Glycine(s) 39 Alanine(s) 13 Lysine(s) 11 Aspartate(s) 34 Arginine(s) 32 Glutamine(s) 14 Serine(s) 8 Methionine(s) 8 Tryptophan(s) 4 Phenylalanine(s) 4 Tyrosine(s) 2 Cysteine(s) 41 Leucine(s) 2 Histidine(s) 8 Proline(s) 1 Asparagine(s) 24 Valine(s) 12 Threonine(s) 2 Isoleucine(s) 1585 ATP-energy(c) 17 Proton-gradient(c) | 1 ApoE(c) 112 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 22 | - | - | 1 |
| 335 Plasminogen | Plasminogen | MCES AAA | de novo synthesis and export of Plasminogen | 56 Glutamate(s) 62 Glycine(s) 37 Alanine(s) 49 Lysine(s) 36 Aspartate(s) 42 Arginine(s) 31 Glutamine(s) 56 Serine(s) 11 Methionine(s) 19 Tryptophan(s) 21 Phenylalanine(s) 30 Tyrosine(s) 48 Cysteine(s) 48 Leucine(s) 24 Histidine(s) 69 Proline(s) 40 Asparagine(s) 48 Valine(s) 61 Threonine(s) 22 Isoleucine(s) 4050 ATP-energy(c) | 1 Plasminogen(s) 3 Proton-gradient(c) 296 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |
| 336 Prothrombin | Prothrombin | MCES AAA | de novo synthesis and export of Prothrombin | 51 Glutamate(s) 49 Glycine(s) 42 Alanine(s) 29 Lysine(s) 35 Aspartate(s) 44 Arginine(s) 26 Glutamine(s) 38 Serine(s) 9 Methionine(s) 14 Tryptophan(s) 21 Phenylalanine(s) 21 Tyrosine(s) 26 Cysteine(s) 51 Leucine(s) 13 Histidine(s) 33 Proline(s) 25 Asparagine(s) 37 Valine(s) 36 Threonine(s) 22 Isoleucine(s) 3110 ATP-energy(c) 17 Proton-gradient(c) | 1 Prothrombin(s) 239 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 337 ApoTransferin | ApoTransferin | MCES AAA | de novo synthesis and export of ApoTransferin | 42 Glutamate(s) 52 Glycine(s) 61 Alanine(s) 58 Lysine(s) 45 Aspartate(s) 27 Arginine(s) 17 Glutamine(s) 41 Serine(s) 10 Methionine(s) 8 Tryptophan(s) 28 Phenylalanine(s) 26 Tyrosine(s) 40 Cysteine(s) 65 Leucine(s) 19 Histidine(s) 32 Proline(s) 34 Asparagine(s) 48 Valine(s) 30 Threonine(s) 15 Isoleucine(s) 3490 ATP-energy(c) 27 Proton-gradient(c) | 1 ApoTransferin(s) 265 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |
| 338 Haptoglobin | Haptoglobin | MCES AAA | de novo synthesis and export of Haptoglobin | 25 Glutamate(s) 31 Glycine(s) 30 Alanine(s) 35 Lysine(s) 25 Aspartate(s) 9 Arginine(s) 17 Glutamine(s) 18 Serine(s) 5 Methionine(s) 8 Tryptophan(s) 8 Phenylalanine(s) 21 Tyrosine(s) 12 Cysteine(s) 31 Leucine(s) 13 Histidine(s) 21 Proline(s) 21 Asparagine(s) 36 Valine(s) 22 Threonine(s) 18 Isoleucine(s) 2030 ATP-energy(c) 9 Proton-gradient(c) | 1 Haptoglobin(s) 175 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 23 | - | - | 1 |
| 339 Collagen ADIPO(c) synthesis | Collagen ADIPO(c) | MCES AAA | test synthesis of Collagen ADIPO c | 12 Glutamate(s) 39 Glycine(s) 12 Alanine(s) 12 Lysine(s) 15 Aspartate(s) 7 Arginine(s) 10 Glutamine(s) 7 Serine(s) 5 Methionine(s) 2 Tryptophan(s) 10 Phenylalanine(s) 14 Tyrosine(s) 2 Cysteine(s) 23 Leucine(s) 8 Histidine(s) 17 Proline(s) 11 Asparagine(s) 14 Valine(s) 15 Threonine(s) 9 Isoleucine(s) 1220 ATP-energy(c) 28 Proton-gradient(c) | 1 Collagen ADIPO(c) 104 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 340 Collagen BGH3(c) synthesis | Collagen BGH3(c) | MCES AAA | test synthesis of Collagen BGH3 c | 42 Glutamate(s) 48 Glycine(s) 61 Alanine(s) 33 Lysine(s) 27 Aspartate(s) 37 Arginine(s) 22 Glutamine(s) 41 Serine(s) 14 Methionine(s) 2 Tryptophan(s) 16 Phenylalanine(s) 19 Tyrosine(s) 11 Cysteine(s) 87 Leucine(s) 19 Histidine(s) 31 Proline(s) 40 Asparagine(s) 47 Valine(s) 46 Threonine(s) 40 Isoleucine(s) 3415 ATP-energy(c) 8 Proton-gradient(c) | 1 Collagen BGH3(c) 304 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 341 Collagen C43BP(c) synthesis | Collagen C43BP(c) | MCES AAA | test synthesis of Collagen C43BP c | 54 Glutamate(s) 33 Glycine(s) 37 Alanine(s) 40 Lysine(s) 45 Aspartate(s) 34 Arginine(s) 23 Glutamine(s) 58 Serine(s) 10 Methionine(s) 14 Tryptophan(s) 22 Phenylalanine(s) 19 Tyrosine(s) 12 Cysteine(s) 38 Leucine(s) 19 Histidine(s) 24 Proline(s) 29 Asparagine(s) 49 Valine(s) 35 Threonine(s) 29 Isoleucine(s) 3120 ATP-energy(c) 4 Proton-gradient(c) | 1 Collagen C43BP(c) 350 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 342 Collagen CCBE1(c) synthesis | Collagen CCBE1(c) | MCES AAA | test synthesis of Collagen CCBE1 c | 26 Glutamate(s) 52 Glycine(s) 20 Alanine(s) 23 Lysine(s) 24 Aspartate(s) 29 Arginine(s) 13 Glutamine(s) 23 Serine(s) 8 Methionine(s) 1 Tryptophan(s) 10 Phenylalanine(s) 17 Tyrosine(s) 21 Cysteine(s) 32 Leucine(s) 8 Histidine(s) 47 Proline(s) 9 Asparagine(s) 9 Valine(s) 22 Threonine(s) 12 Isoleucine(s) 2030 ATP-energy(c) 43 Proton-gradient(c) | 1 Collagen CCBE1(c) 160 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 343 Collagen CD36(c) synthesis | Collagen CD36(c) | MCES AAA | test synthesis of Collagen CD36 c | 24 Glutamate(s) 28 Glycine(s) 25 Alanine(s) 30 Lysine(s) 20 Aspartate(s) 17 Arginine(s) 19 Glutamine(s) 33 Serine(s) 11 Methionine(s) 5 Trypto-phan(s) 27 Phenylalanine(s) 20 Tyrosine(s) 10 Cysteine(s) 41 Leucine(s) 4 Histidine(s) 23 Proline(s) 31 Asparagine(s) 44 Valine(s) 25 Threonine(s) 35 Isoleucine(s) 2360 ATP-energy(c) | 3 Proton-gradient(c) 1 Collagen CD36(c) 253 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 344 Collagen CO1A1(c) synthesis | Collagen CO1A1(c) | MCES AAA | test synthesis of Collagen CO1A1 c | 75 Glutamate(s) 391 Glycine(s) 139 Alanine(s) 57 Lysine(s) 66 Aspartate(s) 71 Arginine(s) 49 Glutamine(s) 60 Serine(s) 13 Methionine(s) 6 Trypto-phan(s) 27 Phenylalanine(s) 13 Tyrosine(s) 18 Cysteine(s) 48 Leucine(s) 9 Histidine(s) 278 Proline(s) 28 Asparagine(s) 47 Valine(s) 45 Threonine(s) 24 Isoleucine(s) 7320 ATP-energy(c) 363 Proton-gradient(c) | 1 Collagen CO1A1(c) 373 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 345 Collagen CO1A2(c) synthesis | Collagen CO1A2(c) | MCES AAA | test synthesis of Collagen CO1A2 c | 66 Glutamate(s) 381 Glycine(s) 129 Alanine(s) 50 Lysine(s) 43 Aspartate(s) 72 Arginine(s) 33 Glutamine(s) 52 Serine(s) 10 Methionine(s) 5 Trypto-phan(s) 22 Phenylalanine(s) 16 Tyrosine(s) 9 Cysteine(s) 61 Leucine(s) 15 Histidine(s) 232 Proline(s) 41 Asparagine(s) 55 Valine(s) 42 Threonine(s) 32 Isoleucine(s) 6830 ATP-energy(c) 340 Proton-gradient(c) | 1 Collagen CO1A2(c) 356 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 346 Collagen $CO_2$A1(c) synthesis | Collagen $CO_2$A1(c) | MCES AAA | test synthesis of Collagen $CO_2$A1 c | 79 Glutamate(s) 406 Glycine(s) 134 Alanine(s) 67 Lysine(s) 62 Aspartate(s) 72 Arginine(s) 60 Glutamine(s) 48 Serine(s) 16 Methionine(s) 7 Tryptophan(s) 25 Phenylalanine(s) 10 Tyrosine(s) 19 Cysteine(s) 56 Leucine(s) 8 Histidine(s) 270 Proline(s) 32 Asparagine(s) 38 Valine(s) 44 Threonine(s) 34 Isoleucine(s) 7435 ATP-energy(c) 374 Proton-gradient(c) | 1 Collagen $CO_2$A1(c) 362 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 347 Collagen CO3A1(c) synthesis | Collagen CO3A1(c) | MCES AAA | test synthesis of Collagen CO3A1 c | 74 Glutamate(s) 413 Glycine(s) 115 Alanine(s) 62 Lysine(s) 55 Aspartate(s) 60 Arginine(s) 42 Glutamine(s) 73 Serine(s) 17 Methionine(s) 7 Tryptophan(s) 23 Phenylalanine(s) 15 Tyrosine(s) 22 Cysteine(s) 48 Leucine(s) 15 Histidine(s) 281 Proline(s) 41 Asparagine(s) 36 Valine(s) 31 Threonine(s) 36 Isoleucine(s) 7330 ATP-energy(c) 372 Proton-gradient(c) | 1 Collagen CO3A1(c) 397 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 348 Collagen CO4A1(c) synthesis | Collagen CO4A1(c) | MCES AAA | test synthesis of Collagen CO4A1 c | 70 Glutamate(s) 478 Glycine(s) 58 Alanine(s) 93 Lysine(s) 58 Aspartate(s) 45 Arginine(s) 73 Glutamine(s) 72 Serine(s) 31 Methionine(s) 6 Tryptophan(s) 46 Phenylalanine(s) 18 Tyrosine(s) 20 Cysteine(s) 92 Leucine(s) 16 Histidine(s) 324 Proline(s) 16 Asparagine(s) 51 Valine(s) 44 Threonine(s) 58 Isoleucine(s) 8345 ATP-energy(c) 462 Proton-gradient(c) | 1 Collagen CO4A1(c) 431 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 349 Collagen CO4A2(c) synthesis | Collagen CO4A2(c) | MCES AAA | test synthesis of Collagen CO4A2 c | 60 Glutamate(s) 473 Glycine(s) 82 Alanine(s) 81 Lysine(s) 82 Aspartate(s) 79 Arginine(s) 62 Glutamine(s) 64 Serine(s) 25 Methionine(s) 9 Tryptophan(s) 57 Phenylalanine(s) 28 Tyrosine(s) 21 Cysteine(s) 102 Leucine(s) 19 Histidine(s) 286 Proline(s) 18 Asparagine(s) 50 Valine(s) 51 Threonine(s) 63 Isoleucine(s) 8560 ATP-energy(c) 455 Proton-gradient(c) | 1 Collagen CO4A2(c) 471 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 350 Collagen CO4A3(c) synthesis | Collagen CO4A3(c) | MCES AAA | test synthesis of Collagen CO4A3 c | 67 Glutamate(s) 455 Glycine(s) 69 Alanine(s) 89 Lysine(s) 53 Aspartate(s) 65 Arginine(s) 48 Glutamine(s) 78 Serine(s) 29 Methionine(s) 6 Tryptophan(s) 46 Phenylalanine(s) 18 Tyrosine(s) 24 Cysteine(s) 106 Leucine(s) 19 Histidine(s) 320 Proline(s) 28 Asparagine(s) 40 Valine(s) 59 Threonine(s) 51 Isoleucine(s) 8350 ATP-energy(c) 427 Proton-gradient(c) | 1 Collagen CO4A3(c) 430 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 351 Collagen CO4A4(c) synthesis | Collagen CO4A4(c) | MCES AAA | test synthesis of Collagen CO4A4 c | 58 Glutamate(s) 464 Glycine(s) 69 Alanine(s) 83 Lysine(s) 72 Aspartate(s) 70 Arginine(s) 48 Glutamine(s) 76 Serine(s) 24 Methionine(s) 9 Tryptophan(s) 45 Phenylalanine(s) 23 Tyrosine(s) 32 Cysteine(s) 101 Leucine(s) 33 Histidine(s) 345 Proline(s) 15 Asparagine(s) 50 Valine(s) 30 Threonine(s) 43 Isoleucine(s) 8450 ATP-energy(c) 449 Proton-gradient(c) | 1 Collagen CO4A4(c) 456 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 352 Collagen CO4A5(c) synthesis | Collagen CO4A5(c) | MCES AAA | test synthesis of Collagen CO4A5 c | 61 Glutamate(s) 478 Glycine(s) 47 Alanine(s) 80 Lysine(s) 54 Aspartate(s) 37 Arginine(s) 73 Glutamine(s) 64 Serine(s) 26 Methionine(s) 5 Tryptophan(s) 41 Phenylalanine(s) 13 Tyrosine(s) 20 Cysteine(s) 112 Leucine(s) 13 Histidine(s) 391 Proline(s) 32 Asparagine(s) 31 Valine(s) 38 Threonine(s) 69 Isoleucine(s) 8425 ATP-energy(c) 446 Proton-gradient(c) | 1 Collagen CO4A5(c) 403 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 353 Collagen CO4A6(c) synthesis | Collagen CO4A6(c) | MCES AAA | test synthesis of Collagen CO4A6 c | 57 Glutamate(s) 463 Glycine(s) 60 Alanine(s) 96 Lysine(s) 52 Aspartate(s) 47 Arginine(s) 65 Glutamine(s) 98 Serine(s) 25 Methionine(s) 8 Tryptophan(s) 55 Phenylalanine(s) 15 Tyrosine(s) 21 Cysteine(s) 140 Leucine(s) 17 Histidine(s) 279 Proline(s) 26 Asparagine(s) 51 Valine(s) 53 Threonine(s) 63 Isoleucine(s) 8455 ATP-energy(c) 437 Proton-gradient(c) | 1 Collagen CO4A6(c) 463 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 354 Collagen CO5A1(c) synthesis | Collagen CO5A1(c) | MCES AAA | test synthesis of Collagen CO5A1 c | 120 Glutamate(s) 429 Glycine(s) 92 Alanine(s) 98 Lysine(s) 105 Aspartate(s) 70 Arginine(s) 74 Glutamine(s) 70 Serine(s) 23 Methionine(s) 7 Tryptophan(s) 39 Phenylalanine(s) 40 Tyrosine(s) 12 Cysteine(s) 98 Leucine(s) 17 Histidine(s) 334 Proline(s) 34 Asparagine(s) 54 Valine(s) 70 Threonine(s) 52 Isoleucine(s) 9190 ATP-energy(c) 395 Proton-gradient(c) | 1 Collagen CO5A1(c) 550 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 355 Collagen CO5A2(c) synthesis | Collagen CO5A2(c) | MCES AAA | test synthesis of Collagen CO5A2 c | 76 Glutamate(s) 402 Glycine(s) 83 Alanine(s) 61 Lysine(s) 69 Aspartate(s) 74 Arginine(s) 60 Glutamine(s) 63 Serine(s) 24 Methionine(s) 6 Tryptophan(s) 20 Phenylalanine(s) 11 Tyrosine(s) 17 Cysteine(s) 62 Leucine(s) 17 Histidine(s) 270 Proline(s) 36 Asparagine(s) 58 Valine(s) 51 Threonine(s) 39 Isoleucine(s) 7495 ATP-energy(c) 366 Proton-gradient(c) | 1 Collagen CO5A2(c) 412 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 356 Collagen CO5A3(c) synthesis | Collagen CO5A3(c) | MCES AAA | test synthesis of Collagen CO5A3 c | 101 Glutamate(s) 429 Glycine(s) 102 Alanine(s) 86 Lysine(s) 76 Aspartate(s) 84 Arginine(s) 78 Glutamine(s) 69 Serine(s) 12 Methionine(s) 8 Tryptophan(s) 46 Phenylalanine(s) 11 Tyrosine(s) 12 Cysteine(s) 122 Leucine(s) 23 Histidine(s) 290 Proline(s) 24 Asparagine(s) 67 Valine(s) 67 Threonine(s) 38 Isoleucine(s) 8725 ATP-energy(c) 405 Proton-gradient(c) | 1 Collagen CO5A3(c) 475 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 357 Collagen CO6A1(c) synthesis | Collagen CO6A1(c) | MCES AAA | test synthesis of Collagen CO6A1 c | 68 Glutamate(s) 156 Glycine(s) 77 Alanine(s) 54 Lysine(s) 71 Aspartate(s) 60 Arginine(s) 42 Glutamine(s) 54 Serine(s) 11 Methionine(s) 4 Tryptophan(s) 33 Phenylalanine(s) 28 Tyrosine(s) 20 Cysteine(s) 71 Leucine(s) 14 Histidine(s) 89 Proline(s) 28 Asparagine(s) 65 Valine(s) 41 Threonine(s) 42 Isoleucine(s) 5140 ATP-energy(c) 128 Proton-gradient(c) | 1 Collagen CO6A1(c) 427 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 358 Collagen CO6A2(c) synthesis | Collagen CO6A2(c) | MCES AAA | test synthesis of Collagen CO6A2 c | 65 Glutamate(s) 155 Glycine(s) 60 Alanine(s) 53 Lysine(s) 71 Aspartate(s) 68 Arginine(s) 45 Glutamine(s) 54 Serine(s) 13 Methionine(s) 5 Tryptophan(s) 39 Phenylalanine(s) 18 Tyrosine(s) 21 Cysteine(s) 66 Leucine(s) 20 Histidine(s) 89 Proline(s) 30 Asparagine(s) 60 Valine(s) 45 Threonine(s) 42 Isoleucine(s) 5095 ATP-energy(c) 125 Proton-gradient(c) | 1 Collagen CO6A2(c) 425 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 359 Collagen CO6A3(c) synthesis | Collagen CO6A3(c) | MCES AAA | test synthesis of Collagen CO6A3 c | 183 Glutamate(s) 303 Glycine(s) 235 Alanine(s) 158 Lysine(s) 183 Aspartate(s) 189 Arginine(s) 147 Glutamine(s) 217 Serine(s) 37 Methionine(s) 6 Tryptophan(s) 149 Phenylalanine(s) 62 Tyrosine(s) 30 Cysteine(s) 282 Leucine(s) 45 Histidine(s) 209 Proline(s) 130 Asparagine(s) 292 Valine(s) 167 Threonine(s) 153 Isoleucine(s) 15885 ATP-energy(c) 173 Proton-gradient(c) | 1 Collagen CO6A3(c) 1450 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 360 Collagen CO6A5(c) synthesis | Collagen CO6A5(c) | MCES AAA | test synthesis of Collagen CO6A5 c | 154 Glutamate(s) 244 Glycine(s) 138 Alanine(s) 179 Lysine(s) 164 Aspartate(s) 124 Arginine(s) 143 Glutamine(s) 188 Serine(s) 55 Methionine(s) 12 Tryptophan(s) 132 Phenylalanine(s) 71 Tyrosine(s) 36 Cysteine(s) 223 Leucine(s) 58 Histidine(s) 108 Proline(s) 130 Asparagine(s) 160 Valine(s) 135 Threonine(s) 161 Isoleucine(s) 13075 ATP-energy(c) 114 Proton-gradient(c) | 1 Collagen CO6A5(c) 1266 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 361 Collagen CO6A6(c) synthesis | Collagen CO6A6(c) | MCES AAA | test synthesis of Collagen CO6A6 c | 150 Glutamate(s) 230 Glycine(s) 149 Alanine(s) 152 Lysine(s) 137 Aspartate(s) 121 Arginine(s) 95 Glutamine(s) 170 Serine(s) 47 Methionine(s) 6 Trypto-phan(s) 109 Phenylalanine(s) 47 Tyrosine(s) 29 Cysteine(s) 180 Leucine(s) 48 Histidine(s) 108 Proline(s) 92 Asparagine(s) 157 Valine(s) 103 Threonine(s) 133 Isoleucine(s) 11315 ATP-energy(c) 138 Proton-gradient(c) | 1 Collagen CO6A6(c) 1078 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 362 Collagen CO7A1(c) synthesis | Collagen CO7A1(c) | MCES AAA | test synthesis of Collagen CO7A1 c | 187 Glutamate(s) 627 Glycine(s) 193 Alanine(s) 93 Lysine(s) 145 Aspartate(s) 217 Arginine(s) 105 Glutamine(s) 166 Serine(s) 18 Methionine(s) 19 Trypto-phan(s) 39 Phenylalanine(s) 36 Tyrosine(s) 17 Cysteine(s) 212 Leucine(s) 28 Histidine(s) 426 Proline(s) 27 Asparagine(s) 201 Valine(s) 132 Threonine(s) 56 Isoleucine(s) 14720 ATP-energy(c) 600 Proton-gradient(c) | 1 Collagen CO7A1(c) 921 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 363 Collagen CO8A1(c) synthesis | Collagen CO8A1(c) | MCES AAA | test synthesis of Collagen CO8A1 c | 26 Glutamate(s) 190 Glycine(s) 33 Alanine(s) 47 Lysine(s) 11 Aspartate(s) 13 Arginine(s) 38 Glutamine(s) 11 Serine(s) 23 Methionine(s) 1 Trypto-phan(s) 17 Phenylalanine(s) 22 Tyrosine(s) 2 Cysteine(s) 53 Leucine(s) 11 Histidine(s) 167 Proline(s) 8 Asparagine(s) 30 Valine(s) 8 Threonine(s) 33 Isoleucine(s) 3720 ATP-energy(c) 182 Proton-gradient(c) | 1 Collagen CO8A1(c) 172 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 364 Collagen CO8A2(c) synthesis | Collagen CO8A2(c) | MCES AAA | test synthesis of Collagen CO8A2 c | 24 Glutamate(s) 193 Glycine(s) 42 Alanine(s) 28 Lysine(s) 18 Aspartate(s) 21 Arginine(s) 25 Glutamine(s) 22 Serine(s) 9 Methionine(s) 2 Tryptophan(s) 14 Phenylalanine(s) 16 Tyrosine(s) 3 Cysteine(s) 59 Leucine(s) 8 Histidine(s) 145 Proline(s) 9 Asparagine(s) 31 Valine(s) 22 Threonine(s) 12 Isoleucine(s) 3515 ATP-energy(c) 184 Proton-gradient(c) | 1 Collagen CO8A2(c) 159 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 365 Collagen CO9A1(c) synthesis | Collagen CO9A1(c) | MCES AAA | test synthesis of Collagen CO9A1 c | 47 Glutamate(s) 217 Glycine(s) 47 Alanine(s) 42 Lysine(s) 39 Aspartate(s) 54 Arginine(s) 39 Glutamine(s) 42 Serine(s) 12 Methionine(s) 6 Tryptophan(s) 22 Phenylalanine(s) 6 Tyrosine(s) 11 Cysteine(s) 57 Leucine(s) 8 Histidine(s) 153 Proline(s) 20 Asparagine(s) 37 Valine(s) 26 Threonine(s) 36 Isoleucine(s) 4605 ATP-energy(c) 197 Proton-gradient(c) | 1 Collagen CO9A1(c) 274 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 366 Collagen CO9A2(c) synthesis | Collagen CO9A2(c) | MCES AAA | test synthesis of Collagen CO9A2 c | 31 Glutamate(s) 203 Glycine(s) 42 Alanine(s) 38 Lysine(s) 24 Aspartate(s) 27 Arginine(s) 34 Glutamine(s) 18 Serine(s) 11 Methionine(s) 4 Phenylalanine(s) 6 Tyrosine(s) 4 Cysteine(s) 28 Leucine(s) 8 Histidine(s) 138 Proline(s) 6 Asparagine(s) 29 Valine(s) 15 Threonine(s) 23 Isoleucine(s) 3445 ATP-energy(c) 197 Proton-gradient(c) | 1 Collagen CO9A2(c) 153 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 21 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 367 Collagen CO9A3(c) synthesis | Collagen CO9A3(c) | MCES AAA | test synthesis of Collagen CO9A3 c | 32 Glutamate(s) 210 Glycine(s) 45 Alanine(s) 29 Lysine(s) 28 Aspartate(s) 32 Arginine(s) 25 Glutamine(s) 25 Serine(s) 6 Methionine(s) 4 Phenylalanine(s) 2 Tyrosine(s) 6 Cysteine(s) 49 Leucine(s) 4 Histidine(s) 137 Proline(s) 5 Asparagine(s) 20 Valine(s) 11 Threonine(s) 14 Isoleucine(s) 3420 ATP-energy(c) 205 Proton-gradient(c) | 1 Collagen CO9A3(c) 140 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 21 | - | - | - |
| 368 Collagen COAA1(c) synthesis | Collagen COAA1(c) | MCES AAA | test synthesis of Collagen COAA1 c | 22 Glutamate(s) 175 Glycine(s) 36 Alanine(s) 35 Lysine(s) 12 Aspartate(s) 19 Arginine(s) 23 Glutamine(s) 27 Serine(s) 11 Methionine(s) 2 Tryptophan(s) 15 Phenylalanine(s) 21 Tyrosine(s) 1 Cysteine(s) 35 Leucine(s) 10 Histidine(s) 145 Proline(s) 14 Asparagine(s) 26 Valine(s) 24 Threonine(s) 27 Isoleucine(s) 3400 ATP-energy(c) 161 Proton-gradient(c) | 1 Collagen COAA1(c) 177 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 369 Collagen COBA1(c) synthesis | Collagen COBA1(c) | MCES AAA | test synthesis of Collagen COBA1 c | 123 Glutamate(s) 422 Glycine(s) 98 Alanine(s) 106 Lysine(s) 99 Aspartate(s) 68 Arginine(s) 81 Glutamine(s) 73 Serine(s) 24 Methionine(s) 9 Tryptophan(s) 47 Phenylalanine(s) 36 Tyrosine(s) 11 Cysteine(s) 80 Leucine(s) 17 Histidine(s) 287 Proline(s) 37 Asparagine(s) 63 Valine(s) 69 Threonine(s) 56 Isoleucine(s) 9030 ATP-energy(c) 385 Proton-gradient(c) | 1 Collagen COBA1(c) 571 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 370 Collagen COBA2(c) synthesis | Collagen COBA2(c) | MCES AAA | test synthesis of Collagen COBA2 c | 110 Glutamate(s) 428 Glycine(s) 98 Alanine(s) 72 Lysine(s) 79 Aspartate(s) 101 Arginine(s) 87 Glutamine(s) 65 Serine(s) 16 Methionine(s) 3 Tryptophan(s) 31 Phenylalanine(s) 23 Tyrosine(s) 14 Cysteine(s) 111 Leucine(s) 20 Histidine(s) 299 Proline(s) 15 Asparagine(s) 74 Valine(s) 60 Threonine(s) 30 Isoleucine(s) 8680 ATP-energy(c) 413 Proton-gradient(c) | 1 Collagen COBA2(c) 464 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 371 Collagen COCA1(c) synthesis | Collagen COCA1(c) | MCES AAA | test synthesis of Collagen COCA1 c | 194 Glutamate(s) 281 Glycine(s) 159 Alanine(s) 156 Lysine(s) 172 Aspartate(s) 157 Arginine(s) 104 Glutamine(s) 241 Serine(s) 45 Methionine(s) 30 Tryptophan(s) 91 Phenylalanine(s) 113 Tyrosine(s) 21 Cysteine(s) 203 Leucine(s) 31 Histidine(s) 263 Proline(s) 118 Asparagine(s) 270 Valine(s) 266 Threonine(s) 148 Isoleucine(s) 15315 ATP-energy(c) 163 Proton-gradient(c) | 1 Collagen COCA1(c) 1429 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 372 Collagen CODA1(c) synthesis | Collagen CODA1(c) | MCES AAA | test synthesis of Collagen CODA1 c | 44 Glutamate(s) 184 Glycine(s) 49 Alanine(s) 46 Lysine(s) 23 Aspartate(s) 35 Arginine(s) 28 Glutamine(s) 24 Serine(s) 13 Methionine(s) 2 Tryptophan(s) 5 Phenylalanine(s) 3 Tyrosine(s) 8 Cysteine(s) 53 Leucine(s) 11 Histidine(s) 125 Proline(s) 11 Asparagine(s) 17 Valine(s) 17 Threonine(s) 19 Isoleucine(s) 3585 ATP-energy(c) 173 Proton-gradient(c) | 1 Collagen CODA1(c) 167 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 373 Collagen COEA1(c) synthesis | Collagen COEA1(c) | MCES AAA | test synthesis of Collagen COEA1 c | 118 Glutamate(s) 195 Glycine(s) 94 Alanine(s) 86 Lysine(s) 93 Aspartate(s) 74 Arginine(s) 71 Glutamine(s) 133 Serine(s) 33 Methionine(s) 18 Tryptophan(s) 60 Phenylalanine(s) 53 Tyrosine(s) 19 Cysteine(s) 129 Leucine(s) 29 Histidine(s) 156 Proline(s) 58 Asparagine(s) 142 Valine(s) 136 Threonine(s) 99 Isoleucine(s) 8980 ATP-energy(c) 137 Proton-gradient(c) | 1 Collagen COEA1(c) 822 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 374 Collagen COFA1(c) synthesis | Collagen COFA1(c) | MCES AAA | test synthesis of Collagen COFA1 c | 97 Glutamate(s) 221 Glycine(s) 108 Alanine(s) 52 Lysine(s) 58 Aspartate(s) 47 Arginine(s) 40 Glutamine(s) 99 Serine(s) 30 Methionine(s) 10 Tryptophan(s) 43 Phenylalanine(s) 14 Tyrosine(s) 10 Cysteine(s) 112 Leucine(s) 25 Histidine(s) 191 Proline(s) 38 Asparagine(s) 65 Valine(s) 74 Threonine(s) 54 Isoleucine(s) 6940 ATP-energy(c) 183 Proton-gradient(c) | 1 Collagen COFA1(c) 513 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 375 Collagen COGA1(c) synthesis | Collagen COGA1(c) | MCES AAA | test synthesis of Collagen COGA1 c | 92 Glutamate(s) 391 Glycine(s) 85 Alanine(s) 87 Lysine(s) 52 Aspartate(s) 63 Arginine(s) 79 Glutamine(s) 76 Serine(s) 26 Methionine(s) 8 Tryptophan(s) 30 Phenylalanine(s) 13 Tyrosine(s) 32 Cysteine(s) 99 Leucine(s) 19 Histidine(s) 282 Proline(s) 23 Asparagine(s) 63 Valine(s) 43 Threonine(s) 41 Isoleucine(s) 8020 ATP-energy(c) 368 Proton-gradient(c) | 1 Collagen COGA1(c) 449 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 376 Collagen COHA1(c) synthesis | Collagen COHA1(c) | MCES AAA | test synthesis of Collagen COHA1 c | 63 Glutamate(s) 282 Glycine(s) 85 Alanine(s) 60 Lysine(s) 54 Aspartate(s) 68 Arginine(s) 48 Glutamine(s) 178 Serine(s) 33 Methionine(s) 10 Tryptophan(s) 25 Phenylalanine(s) 36 Tyrosine(s) 7 Cysteine(s) 107 Leucine(s) 23 Histidine(s) 204 Proline(s) 31 Asparagine(s) 58 Valine(s) 84 Threonine(s) 41 Isoleucine(s) 7485 ATP-energy(c) 251 Proton-gradient(c) | 1 Collagen COHA1(c) 526 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 377 Collagen COIA1(c) synthesis | Collagen COIA1(c) | MCES AAA | test synthesis of Collagen COIA1 c | 90 Glutamate(s) 302 Glycine(s) 140 Alanine(s) 42 Lysine(s) 74 Aspartate(s) 91 Arginine(s) 67 Glutamine(s) 121 Serine(s) 15 Methionine(s) 21 Tryptophan(s) 57 Phenylalanine(s) 19 Tyrosine(s) 23 Cysteine(s) 148 Leucine(s) 36 Histidine(s) 296 Proline(s) 27 Asparagine(s) 87 Valine(s) 69 Threonine(s) 29 Isoleucine(s) 8770 ATP-energy(c) 275 Proton-gradient(c) | 1 Collagen COIA1(c) 584 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 378 Collagen COJA1(c) synthesis | Collagen COJA1(c) | MCES AAA | test synthesis of Collagen COJA1 c | 67 Glutamate(s) 261 Glycine(s) 52 Alanine(s) 77 Lysine(s) 49 Aspartate(s) 47 Arginine(s) 46 Glutamine(s) 53 Serine(s) 18 Methionine(s) 7 Tryptophan(s) 25 Phenylalanine(s) 16 Tyrosine(s) 14 Cysteine(s) 71 Leucine(s) 16 Histidine(s) 173 Proline(s) 30 Asparagine(s) 33 Valine(s) 30 Threonine(s) 57 Isoleucine(s) 5710 ATP-energy(c) 231 Proton-gradient(c) | 1 Collagen COJA1(c) 367 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 379 Collagen COKA1(c) synthesis | Collagen COKA1(c) | MCES AAA | test synthesis of Collagen COKA1 c | 73 Glutamate(s) 148 Glycine(s) 114 Alanine(s) 38 Lysine(s) 46 Aspartate(s) 85 Arginine(s) 57 Glutamine(s) 107 Serine(s) 14 Methionine(s) 17 Tryptophan(s) 35 Phenylalanine(s) 26 Tyrosine(s) 13 Cysteine(s) 137 Leucine(s) 28 Histidine(s) 128 Proline(s) 11 Asparagine(s) 98 Valine(s) 86 Threonine(s) 23 Isoleucine(s) 6420 ATP-energy(c) 137 Proton-gradient(c) | 1 Collagen COKA1(c) 477 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 380 Collagen COLA1(c) synthesis | Collagen COLA1(c) | MCES AAA | test synthesis of Collagen COLA1 c | 50 Glutamate(s) 181 Glycine(s) 40 Alanine(s) 68 Lysine(s) 48 Aspartate(s) 38 Arginine(s) 51 Glutamine(s) 50 Serine(s) 12 Methionine(s) 4 Tryptophan(s) 29 Phenylalanine(s) 22 Tyrosine(s) 14 Cysteine(s) 66 Leucine(s) 11 Histidine(s) 106 Proline(s) 26 Asparagine(s) 53 Valine(s) 34 Threonine(s) 54 Isoleucine(s) 4785 ATP-energy(c) 155 Proton-gradient(c) | 1 Collagen COLA1(c) 361 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 381 Collagen COLQ(c) synthesis | Collagen COLQ(c) | MCES AAA | test synthesis of Collagen COLQ c | 21 Glutamate(s) 86 Glycine(s) 9 Alanine(s) 22 Lysine(s) 21 Aspartate(s) 25 Arginine(s) 19 Glutamine(s) 27 Serine(s) 14 Methionine(s) 2 Tryptophan(s) 15 Phenylalanine(s) 14 Tyrosine(s) 15 Cysteine(s) 36 Leucine(s) 6 Histidine(s) 69 Proline(s) 11 Asparagine(s) 15 Valine(s) 16 Threonine(s) 12 Isoleucine(s) 2275 ATP-energy(c) 75 Proton-gradient(c) | 1 Collagen COLQ(c) 159 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 382 Collagen COMA1(c) synthesis | Collagen COMA1(c) | MCES AAA | test synthesis of Collagen COMA1 c | 104 Glutamate(s) 395 Glycine(s) 94 Alanine(s) 87 Lysine(s) 70 Aspartate(s) 85 Arginine(s) 62 Glutamine(s) 66 Serine(s) 20 Methionine(s) 6 Tryptophan(s) 34 Phenylalanine(s) 16 Tyrosine(s) 18 Cysteine(s) 101 Leucine(s) 19 Histidine(s) 267 Proline(s) 25 Asparagine(s) 70 Valine(s) 42 Threonine(s) 45 Isoleucine(s) 8130 ATP-energy(c) 370 Proton-gradient(c) | 1 Collagen COMA1(c) 473 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 383 Collagen CONA1(c) synthesis | Collagen CONA1(c) | MCES AAA | test synthesis of Collagen CONA1 c | 36 Glutamate(s) 147 Glycine(s) 43 Alanine(s) 35 Lysine(s) 29 Aspartate(s) 30 Arginine(s) 17 Glutamine(s) 17 Serine(s) 5 Methionine(s) 2 Tryptophan(s) 2 Phenylalanine(s) 2 Tyrosine(s) 6 Cysteine(s) 40 Leucine(s) 3 Histidine(s) 93 Proline(s) 2 Asparagine(s) 15 Valine(s) 8 Threonine(s) 8 Isoleucine(s) 2700 ATP-energy(c) 145 Proton-gradient(c) | 1 Collagen CONA1(c) 122 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 384 Collagen COOA1(c) synthesis | Collagen COOA1(c) | MCES AAA | test synthesis of Collagen COOA1 c | 102 Glutamate(s) 365 Glycine(s) 58 Alanine(s) 104 Lysine(s) 60 Aspartate(s) 66 Arginine(s) 90 Glutamine(s) 90 Serine(s) 24 Methionine(s) 5 Tryptophan(s) 42 Phenylalanine(s) 30 Tyrosine(s) 15 Cysteine(s) 128 Leucine(s) 38 Histidine(s) 207 Proline(s) 54 Asparagine(s) 69 Valine(s) 79 Threonine(s) 88 Isoleucine(s) 8570 ATP-energy(c) 311 Proton-gradient(c) | 1 Collagen COOA1(c) 593 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 385 Collagen COPA1(c) synthesis | Collagen COPA1(c) | MCES AAA | test synthesis of Collagen COPA1 c | 45 Glutamate(s) 167 Glycine(s) 33 Alanine(s) 50 Lysine(s) 28 Aspartate(s) 28 Arginine(s) 32 Glutamine(s) 20 Serine(s) 17 Methionine(s) 1 Tryptophan(s) 5 Phenylalanine(s) 4 Tyrosine(s) 7 Cysteine(s) 41 Leucine(s) 10 Histidine(s) 108 Proline(s) 9 Asparagine(s) 13 Valine(s) 16 Threonine(s) 20 Isoleucine(s) 3270 ATP-energy(c) 158 Proton-gradient(c) | 1 Collagen COPA1(c) 162 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 386 Collagen CORA1(c) synthesis | Collagen CORA1(c) | MCES AAA | test synthesis of Collagen CORA1 c | 67 Glutamate(s) 397 Glycine(s) 110 Alanine(s) 95 Lysine(s) 69 Aspartate(s) 101 Arginine(s) 96 Glutamine(s) 106 Serine(s) 38 Methionine(s) 10 Trypto-phan(s) 49 Phenylalanine(s) 17 Tyrosine(s) 15 Cysteine(s) 134 Leucine(s) 31 Histidine(s) 303 Proline(s) 21 Asparagine(s) 70 Valine(s) 87 Threonine(s) 44 Isoleucine(s) 9300 ATP-energy(c) 376 Proton-gradient(c) | 1 Collagen CORA1(c) 499 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 387 Collagen COSA1(c) synthesis | Collagen COSA1(c) | MCES AAA | test synthesis of Collagen COSA1 c | 73 Glutamate(s) 211 Glycine(s) 42 Alanine(s) 91 Lysine(s) 63 Aspartate(s) 40 Arginine(s) 58 Glutamine(s) 69 Serine(s) 14 Methionine(s) 5 Trypto-phan(s) 38 Phenylalanine(s) 18 Tyrosine(s) 15 Cysteine(s) 66 Leucine(s) 7 Histidine(s) 129 Proline(s) 27 Asparagine(s) 53 Valine(s) 45 Threonine(s) 61 Isoleucine(s) 5625 ATP-energy(c) 184 Proton-gradient(c) | 1 Collagen COSA1(c) 429 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 388 Collagen CTHR1(c) synthesis | Collagen CTHR1(c) | MCES AAA | test synthesis of Collagen CTHR1 c | 15 Glutamate(s) 29 Glycine(s) 15 Alanine(s) 11 Lysine(s) 8 Aspartate(s) 15 Arginine(s) 10 Glutamine(s) 23 Serine(s) 4 Methionine(s) 5 Tryptophan(s) 6 Phenylalanine(s) 6 Tyrosine(s) 10 Cysteine(s) 24 Leucine(s) 1 Histidine(s) 18 Proline(s) 10 Asparagine(s) 9 Valine(s) 9 Threonine(s) 15 Isoleucine(s) 1215 ATP-energy(c) 19 Proton-gradient(c) | 1 Collagen CTHR1(c) 108 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 389 Collagen EMID2(c) synthesis | Collagen EMID2(c) | MCES AAA | test synthesis of Collagen EMID2 c | 24 Glutamate(s) 65 Glycine(s) 38 Alanine(s) 12 Lysine(s) 16 Aspartate(s) 28 Arginine(s) 18 Glutamine(s) 29 Serine(s) 6 Methionine(s) 5 Tryptophan(s) 4 Phenylalanine(s) 8 Tyrosine(s) 13 Cysteine(s) 39 Leucine(s) 7 Histidine(s) 68 Proline(s) 10 Asparagine(s) 21 Valine(s) 23 Threonine(s) 7 Isoleucine(s) 2205 ATP-energy(c) 55 Proton-gradient(c) | 1 Collagen EMID2(c) 144 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 390 Collagen FCN1(c) synthesis | Collagen FCN1(c) | MCES AAA | test synthesis of Collagen FCN1 c | 16 Glutamate(s) 46 Glycine(s) 29 Alanine(s) 21 Lysine(s) 21 Aspartate(s) 14 Arginine(s) 10 Glutamine(s) 21 Serine(s) 7 Methionine(s) 7 Tryptophan(s) 13 Phenylalanine(s) 12 Tyrosine(s) 8 Cysteine(s) 29 Leucine(s) 7 Histidine(s) 15 Proline(s) 15 Asparagine(s) 18 Valine(s) 11 Threonine(s) 6 Isoleucine(s) 1630 ATP-energy(c) 31 Proton-gradient(c) | 1 Collagen FCN1(c) 144 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 391 Collagen FCN2(c) synthesis | Collagen FCN2(c) | MCES AAA | test synthesis of Collagen FCN2 c | 13 Glutamate(s) 43 Glycine(s) 23 Alanine(s) 16 Lysine(s) 21 Aspartate(s) 16 Arginine(s) 9 Glutamine(s) 16 Serine(s) 6 Methionine(s) 8 Tryptophan(s) 14 Phenylalanine(s) 11 Tyrosine(s) 8 Cysteine(s) 29 Leucine(s) 6 Histidine(s) 19 Proline(s) 17 Asparagine(s) 17 Valine(s) 17 Threonine(s) 4 Isoleucine(s) 1565 ATP-energy(c) 26 Proton-gradient(c) | 1 Collagen FCN2(c) 135 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 392 Collagen FCN3(c) synthesis | Collagen FCN3(c) | MCES AAA | test synthesis of Collagen FCN3 c | 18 Glutamate(s) 38 Glycine(s) 20 Alanine(s) 7 Lysine(s) 13 Aspartate(s) 20 Arginine(s) 10 Glutamine(s) 23 Serine(s) 5 Methionine(s) 10 Tryptophan(s) 11 Phenylalanine(s) 10 Tyrosine(s) 9 Cysteine(s) 35 Leucine(s) 10 Histidine(s) 23 Proline(s) 12 Asparagine(s) 13 Valine(s) 9 Threonine(s) 3 Isoleucine(s) 1495 ATP-energy(c) 26 Proton-gradient(c) | 1 Collagen FCN3(c) 132 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 393 Collagen FMOD(c) synthesis | Collagen FMOD(c) | MCES AAA | test synthesis of Collagen FMOD c | 19 Glutamate(s) 17 Glycine(s) 15 Alanine(s) 10 Lysine(s) 20 Aspartate(s) 20 Arginine(s) 18 Glutamine(s) 32 Serine(s) 7 Methionine(s) 4 Tryptophan(s) 12 Phenylalanine(s) 25 Tyrosine(s) 6 Cysteine(s) 55 Leucine(s) 11 Histidine(s) 29 Proline(s) 30 Asparagine(s) 18 Valine(s) 15 Threonine(s) 13 Isoleucine(s) 1880 ATP-energy(c) | 13 Proton-gradient(c) 1 Collagen FMOD(c) 190 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 394 Collagen ITA1(c) synthesis | Collagen ITA1(c) | MCES AAA | test synthesis of Collagen ITA1 c | 73 Glutamate(s) 81 Glycine(s) 60 Alanine(s) 72 Lysine(s) 60 Aspartate(s) 46 Arginine(s) 42 Glutamine(s) 101 Serine(s) 26 Methionine(s) 9 Tryptophan(s) 50 Phenylalanine(s) 41 Tyrosine(s) 27 Cysteine(s) 96 Leucine(s) 22 Histidine(s) 47 Proline(s) 71 Asparagine(s) 90 Valine(s) 86 Threonine(s) 79 Isoleucine(s) 5895 ATP-energy(c) 10 Proton-gradient(c) | 1 Collagen ITA1(c) 623 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 395 Collagen ITA2(c) synthesis | Collagen ITA2(c) | MCES AAA | test synthesis of Collagen ITA2 c | 60 Glutamate(s) 88 Glycine(s) 79 Alanine(s) 59 Lysine(s) 60 Aspartate(s) 32 Arginine(s) 63 Glutamine(s) 102 Serine(s) 21 Methionine(s) 9 Tryptophan(s) 57 Phenylalanine(s) 40 Tyrosine(s) 22 Cysteine(s) 98 Leucine(s) 17 Histidine(s) 47 Proline(s) 75 Asparagine(s) 89 Valine(s) 79 Threonine(s) 84 Isoleucine(s) 5905 ATP-energy(c) 13 Proton-gradient(c) | 1 Collagen ITA2(c) 615 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 396 Collagen LPP3(c) synthesis | Collagen LPP3(c) | MCES AAA | test synthesis of Collagen LPP3 c | 8 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 17 Lysine(s) 13 Aspartate(s) 18 Arginine(s) 10 Glutamine(s) 25 Serine(s) 8 Methionine(s) 1 Tryptophan(s) 20 Phenylalanine(s) 16 Tyrosine(s) 11 Cysteine(s) 32 Leucine(s) 8 Histidine(s) 14 Proline(s) 14 Asparagine(s) 17 Valine(s) 14 Threonine(s) 25 Isoleucine(s) 1555 ATP-energy(c) 4 Proton-gradient(c) | 1 Collagen LPP3(c) 158 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 397 Collagen PCOTH(c) synthesis | Collagen PCOTH(c) | MCES AAA | test synthesis of Collagen PCOTH c | 2 Glutamate(s) 16 Glycine(s) 2 Alanine(s) 4 Lysine(s) 3 Arginine(s) 1 Glutamine(s) 11 Serine(s) 4 Methionine(s) 2 Tryptophan(s) 7 Phenylalanine(s) 1 Cysteine(s) 10 Leucine(s) 26 Proline(s) 2 Asparagine(s) 6 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 535 ATP-energy(c) 14 Proton-gradient(c) | 1 Collagen PCOTH(c) 35 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 19 | - | - | - |
| 398 Collagen SCRB1(c) synthesis | Collagen SCRB1(c) | MCES AAA | test synthesis of Collagen SCRB1 c | 25 Glutamate(s) 45 Glycine(s) 39 Alanine(s) 24 Lysine(s) 14 Aspartate(s) 21 Arginine(s) 17 Glutamine(s) 45 Serine(s) 23 Methionine(s) 11 Tryptophan(s) 32 Phenylalanine(s) 16 Tyrosine(s) 14 Cysteine(s) 59 Leucine(s) 13 Histidine(s) 38 Proline(s) 24 Asparagine(s) 41 Valine(s) 27 Threonine(s) 24 Isoleucine(s) 2760 ATP-energy(c) 21 Proton-gradient(c) | 1 Collagen SCRB1(c) 259 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| 399 Collagen SERPH(c) synthesis | Collagen SERPH(c) | MCES AAA | test synthesis of Collagen SERPH c | 27 Glutamate(s) 24 Glycine(s) 43 Alanine(s) 34 Lysine(s) 24 Aspartate(s) 21 Arginine(s) 13 Glutamine(s) 33 Serine(s) 14 Methionine(s) 4 Tryptophan(s) 16 Phenylalanine(s) 10 Tyrosine(s) 2 Cysteine(s) 54 Leucine(s) 14 Histidine(s) 15 Proline(s) 11 Asparagine(s) 28 Valine(s) 19 Threonine(s) 12 Isoleucine(s) 2090 ATP-energy(c) 13 Proton-gradient(c) | 1 Collagen SERPH(c) 181 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 400 Collagen VWA2(c) synthesis | Collagen VWA2(c) | MCES AAA | test synthesis of Collagen VWA2 c | 44 Glutamate(s) 66 Glycine(s) 66 Alanine(s) 25 Lysine(s) 32 Aspartate(s) 58 Arginine(s) 32 Glutamine(s) 56 Serine(s) 12 Methionine(s) 7 Tryptophan(s) 31 Phenylalanine(s) 13 Tyrosine(s) 27 Cysteine(s) 81 Leucine(s) 17 Histidine(s) 47 Proline(s) 15 Asparagine(s) 72 Valine(s) 36 Threonine(s) 18 Isoleucine(s) 3775 ATP-energy(c) 51 Proton-gradient(c) | 1 Collagen VWA2(c) 332 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 22 | - | - | - |
| **B3.2.2. Lipoproteins** | | | | | | | | | | | | | | | | | |
| 401 VLDL | VLDL | MCES AAA ALFA | de novo synthesis and export of VLDL | 578 Glutamate(s) 333 Glycine(s) 548 Alanine(s) 448 Lysine(s) 310 Aspartate(s) 388 Arginine(s) 454 Glutamine(s) 1060 Serine(s) 135 Methionine(s) 93 Tryptophan(s) 252 Phenylalanine(s) 179 Tyrosine(s) 6452 Glucose-6P(c) 39 Cysteine(s) 3085 Choline(c) 820 Leucine(s) 129 Histidine(s) 227 Proline(s) 254 Asparagine(s) 420 Valine(s) 384 Threonine(s) 370 Ethanolamine(c) 5800 Arachidonate(c) 12708 Palmitate(c) 299 Isoleucine(s) 4290 Farnesyl-PP(r) 15589 Oleate(c) 25.1 Stearate(c) 3107 Linoleate(c) 1949 gamma-Linolenate(c) $1.3{\cdot}10^5$ ATP-energy(c) 6435 NADPH-redox-potential(r) 829.9 CoA-activated acetyl group(r) | 26201 $H_2O$(s) 11761 $P_i$(c) 7005 $CO_2$(s) 1 VLDL(s) 2145 NADH-redox-potential(r) 724 NADH-redox-potential(c) 635 NADPH-redox-potential(c) 179 Proton-gradient(c) 4115 Na-gradient(c) 5120 CoA-activated acetyl group(c) | 66 | - | 35 | - | - | - | - | - | 25 | - | 25 | 3 |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 402 HDL | HDL | MCES AAA ALFA | de novo synthesis and export of HDL | 67.5 $P_i$(c) 60 Glutamate(s) 22 Glycine(s) 46 Alanine(s) 44 Lysine(s) 32 Aspartate(s) 34 Arginine(s) 38 Glutamine(s) 82 Serine(s) 8 Methionine(s) 10 Tryptophan(s) 16 Phenylalanine(s) 14 Tyrosine(s) 72.5 Glucose-6P(c) 165 Choline(c) 82 Leucine(s) 12 Histidine(s) 20 Proline(s) 10 Asparagine(s) 30 Valine(s) 24 Threonine(s) 80 Ethanolamine(c) 85.7 Arachidonate(c) 196.4 Palmitate(c) 40 Farnesyl-PP(r) 143.5 Oleate(c) 7.93 Linoleate(c) 6.38 gamma-Linolenate(c) 4303 ATP-energy(c) 60 NADPH-redox-potential(r) 130 NADPH-redox-potential(c) | 673.9 $H_2O$(s) 80 $CO_2$(s) 1 HDL(s) 20 NADH-redox-potential(r) 50 NADH-redox-potential(c) 14 Proton-gradient(c) 260 Na-gradient(c) 40 CoA-activated acetyl group(c) | 51 | - | 19 | - | - | - | - | - | 23 | - | 14 | 2 |
| **B3.2.3. Ketone bodies** | | | | | | | | | | | | | | | | | |
| 403 Acetoacetate | Acetoacetate | MCES | de novo synthesis and export of Acetoacetate from Palmitate, excreting $CO_2$ | 1 $H_2O$(s) 1 Pyruvate(c) 2 CoA-activated acetyl group(m) | 1 Pyruvate(m) 1 Acetoacetate(s) 1 Proton-gradient(c) | - | 4 | - | - | - | - | - | - | 3 | - | 2 | - |
| 404 (R)-3-Hydroxybutanoate | (R)-3-Hydroxybutanoate(c) | MCES | de novo synthesis and export of (R)-3-Hydroxybutanoate from Palmitate, excreting $CO_2$ | 1 $H_2O$(s) 1 NADH-redox-potential(m) 1 Proton-gradient(m) 2 CoA-activated acetyl group(m) | 1 (R)-3-Hydroxybutanoate(c) | - | 6 | - | - | - | - | - | - | 1 | - | 3 | - |

Continued on next page

B3. Excretion of de novo synthesized substances – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 405 Acetone | Acetone | MCES | de novo synthesis and export of Acetone | 1 $H_2O$(s) 2 CoA-activated acetyl group(m) | 1 $CO_2$(s) 1 Acetone(s) | - | 5 | - | - | - | - | - | - | 3 | - | 2 | - |
| **B3.2.4. Other** | | | | | | | | | | | | | | | | | |
| 406 Heme | Heme(c) | MCES AAA $-Fe^{2+}+$ | de novo synthesis of cytosolic Heme | 2.5 $O_2$(s) 4 Pyruvate(m) 10.5 Glutamate(s) 4 Serine(s) 1.5 Proline(s) 1 $Fe^{2+}$+(s) 4 ATP-energy(c) 1 Proton-gradient(c) 2 Proton-gradient(m) | 14 $H_2O$(s) 14 $CO_2$(s) 1 Heme(c) 4 Aspartate(s) 4 Glutamine(s) 8 NADH-redox-potential(m) 10.5 Na-gradient(c) | 7 | 14 | - | - | - | - | - | - | 10 | - | 12 | - |

## 3.4 B4. clearence " ... degr" simulations

Table 11: B4. clearence " ... degr" simulations

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| **B4.1. amino acids** | | | | | | | | | | | | | | | | | |
| 407 Alanine degr | -1 Alanine(c) | MCES +Urea | Alanine degradation using palmitate excreting urea | 0.5 $H_2O$(s) 1 Alanine(c) 1 ATP-energy(c) 1 ATP-energy(m) | 0.5 Pyruvate(c) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(m) 0.5 CoA-activated acetyl group(m) | 11 | 9 | - | - | - | - | - | - | 2 | - | 2 | - |
| 408 Arginine degr | -1 Arginine(c) | MCES +Urea | Arginine degradation using palmitate excreting urea | 4 $H_2O$(s) 0.5 $O_2$(s) 1 Arginine(c) 2 ATP-energy(c) 1 ATP-energy(m) | 1 $CO_2$(s) 1 Pyruvate(c) 2 Urea(s) 3 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 3 Proton-gradient(m) | 9 | 15 | - | - | - | - | - | - | 4 | - | 11 | - |
| 409 Asparagine degr | -1 Asparagine(c) | MCES +Urea | Asparagine degradation using palmitate excreting urea | 1 $H_2O$(s) 1 Asparagine(c) 2 ATP-energy(c) 2 ATP-energy(m) | 1 Pyruvate(c) 1 Urea(s) 1 NADPH-redox-potential(c) | 10 | 3 | - | - | - | - | - | - | 2 | - | 4 | - |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 410 Aspartate degr | -1 Aspartate(c) | MCES +Urea | Aspartate degradation using palmitate excreting urea | 0.5 $H_2O$(s) 1 Aspartate(c) 1 ATP-energy(c) 1 ATP-energy(m) | 1 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Urea(s) 0.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) 0.5 CoA-activated acetyl group(m) | 10 | 9 | - | - | - | - | - | - | 3 | - | 2 | - | |
| 411 Cysteine degr | -1 Cysteine(c) | MCES +Urea +$H_2S$ | Cysteine degradation using palmitate excreting urea | 0.5 $H_2O$(s) 0.5 Pyruvate(m) 1 Cysteine(c) 1 ATP-energy(c) 1 ATP-energy(m) 1 Proton-gradient(m) | 1 Pyruvate(c) 0.5 Urea(s) 1 $H_2S$(s) 0.5 NADH-redox-potential(c) 0.5 CoA-activated acetyl group(m) | 11 | 6 | - | - | - | - | - | - | 3 | - | 8 | - | |
| 412 Glutamate degr | -1 Glutamate(c) | MCES +Urea | Glutamate degradation using palmitate excreting urea | 1.5 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamate(c) 1 ATP-energy(c) | 1.5 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Pyruvate(m) 0.5 Urea(s) 1.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 5 Proton-gradient(m) | 9 | 13 | - | - | - | - | - | - | 4 | - | 9 | - | |
| 413 Histidine degr | -1 Histidine(c) | MCES +Urea | Histidine degradation using palmitate excreting urea | 2.5 $H_2O$(s) 0.5 $O_2$(s) 1 Histidine(c) 3 ATP-energy(c) 2 ATP-energy(m) 0.5 NADPH-redox-potential(c) | 0.5 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Pyruvate(m) 1.5 Urea(s) 0.5 NADH-redox-potential(c) 1 NADH-redox-potential(m) 4.5 Proton-gradient(m) 1 THF-activated methyl group(c) | 20 | 11 | - | - | - | - | - | - | 4 | - | 12 | - | |
| 414 Glutamine degr | -1 Glutamine(c) | MCES +Urea | Glutamine degradation using palmitate excreting urea | 2 $H_2O$(s) 0.5 $O_2$(s) 1 Glutamine(c) 2 ATP-energy(c) 1 ATP-energy(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Urea(s) 2 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 5 Proton-gradient(m) | 11 | 11 | - | - | - | - | - | - | 4 | - | 7 | - | |
| 415 Leucine degr | -1 Leucine(c) | MCES +Urea | Leucine degradation using palmitate excreting urea | 0.5 $O_2$(s) 0.5 Pyruvate(m) 1 Leucine(c) 1 ATP-energy(c) 1 ATP-energy(m) 1 NADPH-redox-potential(m) | 0.5 $H_2O$(s) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 3 NADH-redox-potential(m) 4 Proton-gradient(m) 3.5 CoA-activated acetyl group(m) | 10 | 18 | - | - | - | - | - | - | 3 | - | 11 | - | |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 416 Lysine degr | -1 Lysine(c) | MCES +Urea | Lysine degradation using palmitate excreting urea | 2 $H_2O$(s) 0.5 $O_2$(s) 1 Pyruvate(m) 1 Lysine(c) 2 ATP-energy(c) 2 ATP-energy(m) 2 NADPH-redox-potential(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Urea(s) 1 NADH-redox-potential(c) 5 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 4 Proton-gradient(m) 2 CoA-activated acetyl group(m) | 11 | 18 | - | - | - | - | - | - | 4 | - | 10 | - |
| 417 Methionine degr | -1 Methionine(c) | MCES +Urea −Serine +$H_2S$ | Methionine degradation using palmitate excreting urea | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Serine(s) 1 Methionine(c) 2 ATP-energy(c) 2 ATP-energy(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Urea(s) 1 $H_2S$(s) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3 Proton-gradient(m) 1 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 15 | 12 | - | - | - | - | - | - | 6 | - | 13 | - |
| 418 Phenylalanine degr | -1 Phenylalanine(c) | MCES +Urea | Phenylalanine degradation using palmitate excreting urea | 0.5 $H_2O$(s) 3 $O_2$(s) 1 Phenylalanine(c) 3 ATP-energy(c) 1 ATP-energy(m) 0.5 NADPH-redox-potential(c) 0.5 Proton-gradient(m) | 1.5 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Pyruvate(m) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 1 NADPH-redox-potential(m) 2 CoA-activated acetyl group(c) | 22 | 6 | - | - | - | - | - | - | 4 | - | 4 | - |
| 419 Proline degr | -1 Proline(c) | MCES +Urea | Proline degradation using palmitate excreting urea | 4.5 $H_2O$(s) 1 Proline(c) 1 ATP-energy(c) 0.5 Proton-gradient(m) | 1.5 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Pyruvate(m) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 2 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 12 | 14 | - | - | - | - | - | - | 3 | - | 7 | - |
| 420 Serine degr | -1 Serine(c) | MCES +Urea | Serine degradation using palmitate excreting urea | 0.5 Pyruvate(m) 1 Serine(c) 1 ATP-energy(c) 1 ATP-energy(m) 0.5 NADPH-redox-potential(c) | 0.5 $H_2O$(s) 1 Pyruvate(c) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 0.5 CoA-activated acetyl group(m) | 19 | 6 | - | - | - | - | - | - | 2 | - | 3 | - |
| 421 Threonine degr | -1 Threonine(c) | MCES +Urea | Threonine degradation using palmitate excreting urea | 0.5 $H_2O$(s) 0.5 $O_2$(s) 1 Threonine(c) 1 ATP-energy(c) 1 ATP-energy(m) 0.5 NADPH-redox-potential(m) | 1.5 $CO_2$(s) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 3 NADH-redox-potential(m) 4 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 11 | 13 | - | - | - | - | - | - | 4 | - | 12 | - |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 422 Tryptophan degr | -1 Tryptophan(c) | MCES +Urea | Tryptophan degradation using palmitate excreting urea | 1 $H_2O$(s) 3.5 $O_2$(s) 1 Pyruvate(m) 1 Tryptophan(c) 3 ATP-energy(c) 2 ATP-energy(m) 2 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 2 $CO_2$(s) 2 Pyruvate(c) 1 Urea(s) 3 NADH-redox-potential(m) 5 Proton-gradient(m) 1 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 23 | 14 | - | - | - | - | - | - | 4 | - | 9 | - |
| 423 Valine degr | -1 Valine(c) | MCES +Urea | Valine degradation using palmitate excreting urea | 2.5 $H_2O$(s) 1 $O_2$(s) 1 Valine(c) 1 ATP-energy(c) | 1.5 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Pyruvate(m) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 3 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 11.5 Proton-gradient(m) | 12 | 18 | - | - | - | - | - | - | 4 | - | 11 | - |
| 424 Glycine degr | -1 Glycine(c) | MCES +Urea −Methionine +$H_2S$ | Glycine degradation using palmitate excreting urea | 0.5 $H_2O$(s) 0.5 Pyruvate(m) 1 Glycine(c) 1 ATP-energy(c) 1 ATP-energy(m) 1 THF-activated methyl group(c) | 1 Pyruvate(c) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 0.5 CoA-activated acetyl group(m) | 22 | 6 | - | - | - | - | - | - | 2 | - | 3 | - |
| 425 Isoleucine degr | -1 Isoleucine(c) | MCES +Urea | Isoleucine degradation using palmitate excreting urea | 1.5 $H_2O$(s) 1 $O_2$(s) 1 Isoleucine(c) 1 ATP-energy(c) 1 ATP-energy(m) | 1.5 $CO_2$(s) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 4 NADH-redox-potential(m) 0.5 NADPH-redox-potential(m) 10 Proton-gradient(m) 2 CoA-activated acetyl group(m) | 10 | 18 | - | - | - | - | - | - | 4 | - | 12 | - |
| 426 Tyrosine degr | -1 Tyrosine(c) | MCES +Urea | Tyrosine degradation using palmitate excreting urea | 1.5 $H_2O$(s) 2 $O_2$(s) 1 Tyrosine(c) 3 ATP-energy(c) 1 ATP-energy(m) 0.5 Proton-gradient(m) | 1.5 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Pyruvate(m) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 0.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 2 CoA-activated acetyl group(c) | 20 | 6 | - | - | - | - | - | - | 4 | - | 4 | - |
| 427 Homocysteine degr | -1 Homocysteine(c) | MCES +Urea −Serine +$H_2S$ | Homocysteine degradation using palmitate excreting urea | 1 $H_2O$(s) 0.5 $O_2$(s) 1 Serine(s) 1 Homocysteine(c) 2 ATP-energy(c) 2 ATP-energy(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Urea(s) 1 $H_2S$(s) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 13 | 12 | - | - | - | - | - | - | 6 | - | 13 | - |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 428 beta-Alanine degr | -1 beta-Alanine(c) | MCES +Urea | beta-Alanine degradation using palmitate excreting urea | 0.5 $H_2O$(s) 1 beta-Alanine(c) 1 ATP-energy(c) 1 ATP-energy(m) 1 Proton-gradient(m) | 0.5 $CO_2$(s) 0.5 Urea(s) 0.5 NADH-redox-potential(c) 1 NADH-redox-potential(m) 0.5 NADPH-redox-potential(m) 1 CoA-activated acetyl group(m) | 10 | 9 | - | - | - | - | - | - | 3 | - | 8 | - |
| 429 Ornithine degr | -1 Ornithine(c) | MCES +Urea | Ornithine degradation using palmitate excreting urea | 3 $H_2O$(s) 0.5 $O_2$(s) 1 Ornithine(c) 2 ATP-energy(c) 1 ATP-energy(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Urea(s) 3 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 3 Proton-gradient(m) | 9 | 15 | - | - | - | - | - | - | 4 | - | 11 | - |
| **B4.2. lipids, fatty acids, lipoproteins** | | | | | | | | | | | | | | | | | |
| 430 LDL degr | -1 LDL | MCES AAA ALFA +Cholesterol(b) | degradation of LDL | 4259 $H_2O$(s) 119 $O_2$(s) 1 LDL(s) 5395 ATP-energy(c) 110 NADH-redox-potential(c) | 473.3 $P_i$(c) 60 $CO_2$(s) 207 Glycine(s) 275 Alanine(s) 357 Lysine(s) 233 Aspartate(s) 150 Arginine(s) 560 Glutamine(s) 552 Serine(s) 79 Methionine(s) 37 Tryptophan(s) 224 Phenylalanine(s) 151 Tyrosine(s) 386.7 Glucose-6P(c) 25 Cysteine(s) 610 Choline(c) 533 Leucine(s) 115 Histidine(s) 139 Proline(s) 247 Asparagine(s) 252 Valine(s) 2195 Cholesterol(b) 300 Threonine(s) 30 Ethanolamine(c) 240.1 Arachidonate(c) 843.9 Palmitate(c) 285 Isoleucine(s) 510.2 Oleate(c) 316 Stearate(c) 1080 Linoleate(c) 252 NADH-redox-potential(m) 320 NADPH-redox-potential(c) 3348 Proton-gradient(m) 110 CoA-activated acetyl group(m) | 48 | 8 | 2 | - | 8 | - | - | - | 23 | 1 | 50 | 2 |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 431 HDL degr | -1 HDL | MCES AAA ALFA +Cholesterol(b) | degradation of HDL | 747.5 $H_2O$(s) 75 Pyruvate(m) 1 HDL(s) 491 ATP-energy(c) 2.5 NADH-redox-potential(c) | 147.5 $P_i$(c) 60 Pyruvate(c) 22 Glycine(s) 46 Alanine(s) 44 Lysine(s) 32 Aspartate(s) 34 Arginine(s) 98 Glutamine(s) 77 Serine(s) 8 Methionine(s) 10 Tryptophan(s) 16 Phenylalanine(s) 14 Tyrosine(s) 72.5 Glucose-6P(c) 165 Choline(c) 82 Leucine(s) 12 Histidine(s) 20 Proline(s) 10 Asparagine(s) 30 Valine(s) 20 Cholesterol(b) 24 Threonine(s) 25 Ethanolamine(c) 49.3 Arachidonate(c) 207.6 Palmitate(c) 39.5 Oleate(c) 69.7 Stearate(c) 71.4 Linoleate(c) 2.5 Palmitolate(c) 75 NADH-redox-potential(m) 150 NADPH-redox-potential(c) 870 Proton-gradient(m) 75 CoA-activated acetyl group(m) | 31 | 3 | 1 | - | - | - | - | - | 19 | 1 | 39 | 2 |
| 432 Oleate degr | -1 Oleate(c) | MCES | degradation of cytosolic oleate | 2 $H_2O$(s) 2.5 $O_2$(s) 1 Oleate(c) 2 ATP-energy(c) | 1 NADH-redox-potential(c) 8 NADH-redox-potential(m) 1 FADH-redox-potential(c) 42 Proton-gradient(m) 9 CoA-activated acetyl group(m) | 9 | 35 | - | - | - | - | - | - | 2 | - | 9 | - |
| 433 Stearate degr | -1 Stearate(c) | MCES | degradation of cytosolic stearate | 3.5 $O_2$(s) 1 Stearate(c) 2 ATP-energy(c) | 8 NADH-redox-potential(m) 1 FADH-redox-potential(c) 42 Proton-gradient(m) 9 CoA-activated acetyl group(m) | 8 | 35 | - | - | - | - | - | - | 1 | - | 9 | - |
| **B4.3. sugars** | | | | | | | | | | | | | | | | | |
| 434 Fructose degr | -1 Fructose | MCES | Fructose degradation | 1 $P_i$(c) 1 Fructose(s) 2 ATP-energy(c) | 1 $H_2O$(s) 1 Glucose-6P(c) | 7 | - | - | - | - | - | - | - | 2 | - | - | - |
| 435 Galactose degr | -1 Galactose | MCES | Galactose degradation | 1 $P_i$(c) 1 Galactose(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Glucose-6P(c) | 5 | - | - | - | - | - | - | - | 2 | - | - | - |
| 436 Mannose degr | -1 Mannose | MCES | Mannose degradation | 1 $P_i$(c) 1 Mannose(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Glucose-6P(c) | 4 | - | - | - | - | - | - | - | 2 | - | - | - |
| **B4.4. Proteins** | | | | | | | | | | | | | | | | | |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 437 Albumin degr | -1 Albumin | MCES AAA | degradation of Albumin | 1 Albumin(s) 304 ATP-energy(c) | 62 Glutamate(s) 13 Glycine(s) 63 Alanine(s) 60 Lysine(s) 36 Aspartate(s) 27 Arginine(s) 20 Glutamine(s) 28 Serine(s) 7 Methionine(s) 2 Tryptophan(s) 35 Phenylalanine(s) 19 Tyrosine(s) 35 Cysteine(s) 64 Leucine(s) 16 Histidine(s) 24 Proline(s) 17 Asparagine(s) 43 Valine(s) 29 Threonine(s) 9 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 438 Antichymotrypsin degr | -1 Antichymotrypsin | MCES AAA | degradation of Antichymotrypsin | 1 Antichymotrypsin(s) 211 ATP-energy(c) | 29 Glutamate(s) 16 Glycine(s) 34 Alanine(s) 26 Lysine(s) 25 Aspartate(s) 16 Arginine(s) 17 Glutamine(s) 30 Serine(s) 14 Methionine(s) 3 Tryptophan(s) 25 Phenylalanine(s) 9 Tyrosine(s) 3 Cysteine(s) 59 Leucine(s) 9 Histidine(s) 16 Proline(s) 19 Asparagine(s) 24 Valine(s) 29 Threonine(s) 20 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 439 Antitrypsin degr | -1 Antitrypsin | MCES AAA | degradation of Antitrypsin | 1 Antitrypsin(s) 209 ATP-energy(c) | 32 Glutamate(s) 24 Glycine(s) 26 Alanine(s) 34 Lysine(s) 24 Aspartate(s) 7 Arginine(s) 18 Glutamine(s) 25 Serine(s) 10 Methionine(s) 3 Tryptophan(s) 27 Phenylalanine(s) 6 Tyrosine(s) 3 Cysteine(s) 51 Leucine(s) 13 Histidine(s) 19 Proline(s) 19 Asparagine(s) 27 Valine(s) 30 Threonine(s) 20 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 440 ApoA1 degr | -1 ApoA1 | MCES AAA | degradation of ApoA1 | 1 ApoA1(s) 133 ATP-energy(c) | 30 Glutamate(s) 11 Glycine(s) 23 Alanine(s) 22 Lysine(s) 16 Aspartate(s) 17 Arginine(s) 19 Glutamine(s) 16 Serine(s) 4 Methionine(s) 5 Tryptophan(s) 8 Phenylalanine(s) 7 Tyrosine(s) 41 Leucine(s) 6 Histidine(s) 10 Proline(s) 5 Asparagine(s) 15 Valine(s) 12 Threonine(s) | 1 | - | - | - | - | - | - | - | 19 | - | - | 1 |
| 441 Fibrinogen degr | -1 Fibrinogen | MCES AAA | degradation of Fibrinogen | 1 Fibrinogen(s) 1337 ATP-energy(c) | 186 Glutamate(s) 262 Glycine(s) 134 Alanine(s) 154 Lysine(s) 176 Aspartate(s) 134 Arginine(s) 110 Glutamine(s) 278 Serine(s) 48 Methionine(s) 60 Tryptophan(s) 98 Phenylalanine(s) 98 Tyrosine(s) 48 Cysteine(s) 166 Leucine(s) 62 Histidine(s) 114 Proline(s) 138 Asparagine(s) 122 Valine(s) 182 Threonine(s) 104 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 442 Haptoglobin degr | -1 Haptoglobin | MCES AAA | degradation of Haptoglobin | 1 Haptoglobin(s) 203 ATP-energy(c) | 25 Glutamate(s) 31 Glycine(s) 30 Alanine(s) 35 Lysine(s) 25 Aspartate(s) 9 Arginine(s) 17 Glutamine(s) 18 Serine(s) 5 Methionine(s) 8 Tryptophan(s) 8 Phenylalanine(s) 21 Tyrosine(s) 12 Cysteine(s) 31 Leucine(s) 13 Histidine(s) 21 Proline(s) 21 Asparagine(s) 36 Valine(s) 22 Threonine(s) 18 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 443 Plasminogen degr | -1 Plasminogen | MCES AAA | degradation of Plasminogen | 1 Plasminogen(s) 405 ATP-energy(c) | 56 Glutamate(s) 62 Glycine(s) 37 Alanine(s) 49 Lysine(s) 36 Aspartate(s) 42 Arginine(s) 31 Glutamine(s) 56 Serine(s) 11 Methionine(s) 19 Tryptophan(s) 21 Phenylalanine(s) 30 Tyrosine(s) 48 Cysteine(s) 48 Leucine(s) 24 Histidine(s) 69 Proline(s) 40 Asparagine(s) 48 Valine(s) 61 Threonine(s) 22 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 444 Prothrombin degr | -1 Prothrombin | MCES AAA | degradation of Prothrombin | 1 Prothrombin(s) 311 ATP-energy(c) | 51 Glutamate(s) 49 Glycine(s) 42 Alanine(s) 29 Lysine(s) 35 Aspartate(s) 44 Arginine(s) 26 Glutamine(s) 38 Serine(s) 9 Methionine(s) 14 Tryptophan(s) 21 Phenylalanine(s) 21 Tyrosine(s) 26 Cysteine(s) 51 Leucine(s) 13 Histidine(s) 33 Proline(s) 25 Asparagine(s) 37 Valine(s) 36 Threonine(s) 22 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 445 ApoTransferin degr | -1 ApoTransferin | MCES AAA | degradation of ApoTransferin | 1 ApoTransferin(s) 349 ATP-energy(c) | 42 Glutamate(s) 52 Glycine(s) 61 Alanine(s) 58 Lysine(s) 45 Aspartate(s) 27 Arginine(s) 17 Glutamine(s) 41 Serine(s) 10 Methionine(s) 8 Tryptophan(s) 28 Phenylalanine(s) 26 Tyrosine(s) 40 Cysteine(s) 65 Leucine(s) 19 Histidine(s) 32 Proline(s) 34 Asparagine(s) 48 Valine(s) 30 Threonine(s) 15 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 21 | - | - | 1 |

Continued on next page

B4. clearence " ... degr" simulations – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 446 ApoB100 degr | -1 ApoB100(l) | MCES AAA | degradation of lysosomal ApoB100 | 1 ApoB100(l) 2280 ATP-energy(c) | 298 Glutamate(s) 207 Glycine(s) 275 Alanine(s) 357 Lysine(s) 233 Aspartate(s) 150 Arginine(s) 230 Glutamine(s) 392 Serine(s) 79 Methionine(s) 37 Tryptophan(s) 224 Phenylalanine(s) 151 Tyrosine(s) 25 Cysteine(s) 533 Leucine(s) 115 Histidine(s) 171 Proline(s) 247 Asparagine(s) 252 Valine(s) 300 Threonine(s) 285 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 20 | - | 23 | 1 |
| 447 Glycogenin degr | -1 Glycogenin(c) | MCES AAA | degradation of cytosolic Glycogenin | 175 ATP-energy(c) 1 Glycogenin(c) | 15 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 18 Lysine(s) 26 Aspartate(s) 12 Arginine(s) 14 Glutamine(s) 31 Serine(s) 8 Methionine(s) 7 Tryptophan(s) 20 Phenylalanine(s) 13 Tyrosine(s) 6 Cysteine(s) 39 Leucine(s) 9 Histidine(s) 15 Proline(s) 12 Asparagine(s) 28 Valine(s) 25 Threonine(s) 12 Isoleucine(s) | 1 | - | - | - | - | - | - | - | 20 | - | - | 1 |
| **B4.5. Ethanol** | | | | | | | | | | | | | | | | | |
| 448 Ethanol degr | -1 Ethanol | MCES | degradation of Ethanol | 1 Ethanol(s) 2 ATP-energy(c) | 2 NADH-redox-potential(c) 1 CoA-activated acetyl group(c) | 8 | - | - | - | - | - | - | - | 1 | - | - | - |
| **B4.6. Other** | | | | | | | | | | | | | | | | | |
| 449 Chitin-component degr | -1 Chitin-component | MCES +Urea | degradation of Chitin-component | 0.5 $H_2O$(s) 1 $P_i$(c) 0.5 Pyruvate(m) 4 ATP-energy(c) 1 ATP-energy(m) 1 Proton-gradient(m) 1 Chitin-component(s) | 0.5 Urea(s) 1 Glucose-6P(c) 0.5 NADH-redox-potential(c) 1 CoA-activated acetyl group(c) 0.5 CoA-activated acetyl group(m) | 16 | 6 | - | - | 1 | - | 1 | - | 2 | - | 10 | - |



# 4 C. Proliferative functions

## 4.1 C1. Cofactors

Table 12: C1. Cofactors

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 450 CoA | CoA(c) | MCES −Pantothenate AAA | de novo synthesis of cytosolic CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 1 CoA(c) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 2 Proton-gradient(c) 5 Na-gradient(c) | 42 | - | - | - | - | - | - | - | 10 | - | - | - |
| 451 $NAD^+$ | $NAD^+$(c) | −Nicotinamide MCES AAA | de novo synthesis of cytosolic $NAD^+$ | 0.33 $P_i$(c) 1 Glycine(s) 1.67 Glucose-6P(c) 2 Asparagine(s) 1 Nicotinamide(s) 16.3 ATP-energy(c) 2 THF-activated methyl group(c) | 3.33 $H_2O$(s) 1 $NAD^+$(c) 1 $CO_2$(s) 2 Pyruvate(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 40 | - | - | - | - | - | - | - | 7 | - | - | - |
| 452 $NADP^+$ | $NADP^+$(c) | −Nicotinamide MCES AAA | de novo synthesis of cytosolic $NADP^+$ | 1.33 $P_i$(c) 1 Glycine(s) 1.67 Glucose-6P(c) 2 Asparagine(s) 1 Nicotinamide(s) 17.3 ATP-energy(c) 2 THF-activated methyl group(c) | 4.33 $H_2O$(s) 1 $NADP^+$(c) 1 $CO_2$(s) 2 Pyruvate(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 41 | - | - | - | - | - | - | - | 7 | - | - | - |
| 453 FAD | FAD(c) | −Riboflavin MCES AAA | de novo synthesis of cytosolic FAD | 1.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Riboflavin(s) 10.2 ATP-energy(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 1 $CO_2$(s) 1 FAD(c) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 2 Na-gradient(c) | 36 | - | - | - | - | - | - | - | 8 | - | - | - |
| 454 Glycogenin | Glycogenin(c) | MCES AAA | de novo synthesis of cytosolic Glycogenin | 15 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 18 Lysine(s) 26 Aspartate(s) 12 Arginine(s) 14 Glutamine(s) 31 Serine(s) 8 Methionine(s) 7 Tryptophan(s) 20 Phenylalanine(s) 13 Tyrosine(s) 6 Cysteine(s) 39 Leucine(s) 9 Histidine(s) 15 Proline(s) 12 Asparagine(s) 28 Valine(s) 25 Threonine(s) 12 Isoleucine(s) 1750 ATP-energy(c) 6 Proton-gradient(c) | 1 Glycogenin(c) 179 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 22 | - | - | 1 |

Continued on next page

C1. Cofactors – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 455 Thioredoxin | Thioredoxin(c) | MCES AAA | de novo synthesis of cytosolic Thioredoxin | 10 Glutamate(s) 5 Glycine(s) 8 Alanine(s) 12 Lysine(s) 7 Aspartate(s) 5 Glutamine(s) 7 Serine(s) 3 Methionine(s) 1 Tryptophan(s) 9 Phenylalanine(s) 1 Tyrosine(s) 5 Cysteine(s) 6 Leucine(s) 1 Histidine(s) 3 Proline(s) 3 Asparagine(s) 11 Valine(s) 4 Threonine(s) 4 Isoleucine(s) 525 ATP-energy(c) 2 Proton-gradient(c) | 1 Thioredoxin(c) 59 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 456 Thioredoxin(m) | mitoThioredoxin(m) | MCES AAA | de novo synthesis of mitochondrial mitoThioredoxin | 6 Glutamate(s) 10 Glycine(s) 11 Alanine(s) 11 Lysine(s) 12 Aspartate(s) 9 Arginine(s) 10 Glutamine(s) 8 Serine(s) 4 Methionine(s) 2 Tryptophan(s) 6 Phenylalanine(s) 2 Tyrosine(s) 3 Cysteine(s) 15 Leucine(s) 3 Histidine(s) 12 Proline(s) 4 Asparagine(s) 17 Valine(s) 12 Threonine(s) 9 Isoleucine(s) 830 ATP-energy(c) 6 Proton-gradient(c) | 1 mitoThioredoxin(m) 72 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 22 | - | 1 | 1 |
| 457 Apo-ACP | Apo-ACP(c) | MCES AAA | de novo synthesis of cytosolic Apo-ACP | 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 2 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 620 ATP-energy(c) 5 Proton-gradient(c) | 1 Apo-ACP(c) 47 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 21 | - | - | 1 |

Continued on next page

C1. Cofactors – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 458 Apo-ACP(m) | mitoApo-ACP(m) | MCES AAA | de novo synthesis of mitochondrial mitoApo-ACP | 22 Pyruvate(m) 8.5 Alanine(s) 7 Lysine(s) 1 Arginine(s) 12 Glutamine(s) 4.5 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 1 Cysteine(s) 10 Leucine(s) 1 Histidine(s) 5 Proline(s) 1 Asparagine(s) 6 Valine(s) 1 Threonine(s) 8 Isoleucine(s) 435 ATP-energy(m) 13 NADPH-redox-potential(m) 34 Proton-gradient(m) | 18.5 NADH-redox-potential(m) 8 Proton-gradient(c) 1 mitoApo-ACP(m) 46.5 Na-gradient(c) 14.5 CoA-activated acetyl group(m) | - | 15 | - | - | - | - | - | - | 18 | - | 17 | 1 |
| 459 THF | THF(c) | −Folate MCES | de novo synthesis of cytosolic THF | 1 Folate(s) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) | 1 THF(c) | 4 | - | - | - | - | - | - | - | 1 | - | - | - |
| 460 Pyridoxal-P | Pyridoxal-P(c) | −Pyridoxine MCES | de novo synthesis of cytosolic Pyridoxal-P | 0.5 $O_2$(s) 1 $P_i$(c) 1 Pyridoxine(s) 1 ATP-energy(c) | 2 $H_2O$(s) 1 Pyridoxal-P(c) | 4 | - | - | - | - | - | - | - | 3 | - | - | - |
| 461 4ppan | D-4-Phospho-pantothenate(c) | −Pantothenate MCES | de novo synthesis of cytosolic D-4-Phosphopantothenate | 1 $P_i$(c) 1 Pantothenate(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 D-4-Phosphopantothenate(c) 1 Na-gradient(c) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 462 thbpt | Tetrahydrobiopterin(c) | −Glutamine(c) MCES | de novo synthesis of cytosolic Tetrahydrobiopterin | 1.83 $H_2O$(s) 1.25 $O_2$(s) 2.5 Glutamine(c) 1.33 Glucose-6P(c) 9.67 ATP-energy(c) | 1.33 $P_i$(c) 4 $CO_2$(s) 2.5 Pyruvate(c) 1 Tetrahydrobiopterin(c) 1.5 ATP-energy(m) 4 NADH-redox-potential(c) 2.5 NADH-redox-potential(m) 1.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) 14 Proton-gradient(m) | 47 | 9 | - | - | - | - | - | - | 3 | - | 12 | - |

Continued on next page

C1. Cofactors – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 463 dhbpt | Dihydrobiopterin(c) | −Glutamine(c) MCES | de novo synthesis of cytosolic Dihydrobiopterin | 1.83 $H_2O$(s) 1.25 $O_2$(s) 2.5 Glutamine(c) 1.33 Glucose-6P(c) 9.67 ATP-energy(c) | 1.33 $P_i$(c) 4 $CO_2$(s) 2.5 Pyruvate(c) 1 Dihydrobiopterin(c) 1.5 ATP-energy(m) 4 NADH-redox-potential(c) 4 NADH-redox-potential(m) 1.5 NADPH-redox-potential(c) 13 Proton-gradient(m) | 46 | 10 | - | - | - | - | - | - | 3 | - | 13 | - |
| 464 mlthf | 5,10-Methylene-THF(c) | −Folate MCES | de novo synthesis of cytosolic 5,10-Methylene-THF | 1 Folate(s) 1 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 1 5,10-Methylene-THF(c) | 5 | - | - | - | - | - | - | - | 1 | - | - | - |
| 465 acgam6p | N-Acetylglucosamine-6P(c) | MCES AAA | de novo synthesis of cytosolic N-Acetylglucosamine-6P | 1 Glutamine(s) 1 Glucose-6P(c) 1 CoA-activated acetyl group(c) | 1 Glutamate(s) 1 N-Acetylglucosamine-6P(c) | 4 | - | - | - | - | - | - | - | 2 | - | - | - |
| 466 THF(m) | THF(m) | −Folate MCES | de novo synthesis of mitochondrial THF | 1 Folate(s) 2 NADPH-redox-potential(m) | 1 THF(m) | - | 3 | - | - | - | - | - | - | 1 | - | 1 | - |
| 467 1fthf | 10-Formyl-THF(c) | −Folate MCES | de novo synthesis of cytosolic 10-Formyl-THF | 1 $H_2O$(s) 1 Folate(s) 1 THF-activated methyl group(c) | 1 10-Formyl-THF(c) | 6 | - | - | - | - | - | - | - | 2 | - | - | - |
| 468 PAPS | PAPS(c) | −Glycine(c) MCES | de novo synthesis of cytosolic PAPS | 1 $P_i$(c) 5 Glycine(c) 1 Glucose-6P(c) 12 ATP-energy(c) 1 activated-sulphur(c) 6 THF-activated methyl group(c) | 1 $H_2O$(s) 4 Pyruvate(c) 1 PAPS(c) 8 NADH-redox-potential(c) 2 NADPH-redox-potential(c) | 45 | - | - | - | - | - | - | - | 1 | - | - | - |
| 469 ametam | S-Adenosylmethioninamine(c) | −Methionine(c) −Glutamine(c) +Glutamate(c) MCES | de novo synthesis of cytosolic S-Adenosylmethioninamine | 5 Glutamine(c) 1 Methionine(c) 1.33 Glucose-6P(c) 1 Activated methyl group(c) 8.67 ATP-energy(c) 3 NADPH-redox-potential(m) 4 Proton-gradient(m) | 0.67 $H_2O$(s) 1.33 $P_i$(c) 5 Glutamate(c) 1 S-Adenosylmethioninamine(c) 2 ATP-energy(m) 4 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 46 | 5 | - | - | - | - | - | - | 1 | - | 8 | - |

Continued on next page

C1. Cofactors – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 470 GSH | GSH(c) | −Cysteine(c) −Glutamine(c) +Glutamate(c) MCES | de novo synthesis of cytosolic GSH | 1 Glutamine(c) 0.5 Glucose-6P(c) 1 Cysteine(c) 1.5 ATP-energy(c) 1 NADH-redox-potential(m) 4 Proton-gradient(m) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 GSH(c) 1 NADH-redox-potential(c) 1 THF-activated methyl group(c) | 16 | 3 | - | - | - | - | - | - | 1 | - | 6 | - | |
| 471 Homocysteine | Homocysteine(c) | −Cysteine(c) MCES | de novo synthesis of cytosolic Homocysteine | 1 $H_2O$(s) 1 Pyruvate(m) 1 Cysteine(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 $CO_2$(s) 1 Pyruvate(c) 1 Homocysteine(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) | 7 | 11 | - | - | - | - | - | - | 2 | - | 4 | - | |

## 4.2 C2. Precursors for macromolecules

Table 13: C2. Precursors for macromolecules

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| **C2.1. For DNA** | | | | | | | | | | | | | | | | | | |
| 472 dATP | dATP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic dATP | 1.67 $P_i$(c) 3 Aspartate(c) 2 Glutamine(c) 1.33 Glucose-6P(c) 8.67 ATP-energy(c) 1 THF-activated methyl group(c) | 3.67 $H_2O$(s) 2 $CO_2$(s) 3 Pyruvate(c) 2 Glutamate(c) 1 dATP(c) 1 NADH-redox-potential(c) 5 NADPH-redox-potential(c) | 44 | - | - | - | - | - | - | - | 2 | - | - | - | |
| 473 dCTP | dCTP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) −$NH_3$(c) MCES | de novo synthesis of cytosolic dCTP | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Aspartate(c) 2 Glutamine(c) 0.83 Glucose-6P(c) 7.17 ATP-energy(c) 1 NADPH-redox-potential(c) | 6.17 $H_2O$(s) 2 Glutamate(c) 1 dCTP(c) 6 Proton-gradient(m) | 26 | - | - | - | - | - | - | - | 2 | - | 6 | - | |
| 474 dGTP | dGTP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic dGTP | 1.67 $P_i$(c) 2 Aspartate(c) 3 Glutamine(c) 1.33 Glucose-6P(c) 9.67 ATP-energy(c) 1 THF-activated methyl group(c) | 2.67 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 3 Glutamate(c) 1 dGTP(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) | 45 | - | - | - | - | - | - | - | 2 | - | - | - | |

Continued on next page

C2. Precursors for macromolecules – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 475 dTTP | dTTP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic dTTP | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Aspartate(c) 1 Glutamine(c) 0.83 Glucose-6P(c) 7.17 ATP-energy(c) 1 ATP-energy(m) 1 NADH-redox-potential(c) 1 THF-activated methyl group(c) | 6.17 $H_2O$(s) 1 Glutamate(c) 1 dTTP(c) 6 Proton-gradient(m) | 30 | 4 | - | - | - | - | - | - | 2 | - | 8 | - |
| **C2.2. For RNA** | | | | | | | | | | | | | | | | | |
| 476 ATP | ATP(c) | −Aspartate(c) +Glutamate(c) −Glutamine(c) MCES | de novo synthesis of cytosolic ATP | 1.67 $P_i$(c) 3 Aspartate(c) 2 Glutamine(c) 1.33 Glucose-6P(c) 8.67 ATP-energy(c) 1 THF-activated methyl group(c) | 2.67 $H_2O$(s) 1 ATP(c) 2 $CO_2$(s) 3 Pyruvate(c) 2 Glutamate(c) 1 NADH-redox-potential(c) 6 NADPH-redox-potential(c) | 42 | - | - | - | - | - | - | - | 2 | - | - | - |
| 477 CTP | CTP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) −$NH_3$(c) MCES | de novo synthesis of cytosolic CTP | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Aspartate(c) 2 Glutamine(c) 0.83 Glucose-6P(c) 7.17 ATP-energy(c) | 5.17 $H_2O$(s) 2 Glutamate(c) 1 CTP(c) 6 Proton-gradient(m) | 23 | - | - | - | - | - | - | - | 2 | - | 6 | - |
| 478 GTP | GTP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic GTP | 1.67 $P_i$(c) 2 Aspartate(c) 3 Glutamine(c) 1.33 Glucose-6P(c) 9.67 ATP-energy(c) 1 THF-activated methyl group(c) | 1.67 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 3 Glutamate(c) 1 GTP(c) 2 NADH-redox-potential(c) 5 NADPH-redox-potential(c) | 43 | - | - | - | - | - | - | - | 2 | - | - | - |
| 479 UTP | UTP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic UTP | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Aspartate(c) 1 Glutamine(c) 0.83 Glucose-6P(c) 6.17 ATP-energy(c) | 5.17 $H_2O$(s) 1 Glutamate(c) 1 UTP(c) 6 Proton-gradient(m) | 22 | - | - | - | - | - | - | - | 2 | - | 6 | - |
| **C2.3. For proteins** | | | | | | | | | | | | | | | | | |
| 480 Alanine | Alanine(c) | −$NH_3$(c) MCES | de novo synthesis of cytosolic Alanine | 1 $NH_3$(c) 1 Pyruvate(c) 1 NADH-redox-potential(m) 2 Proton-gradient(m) | 1 $H_2O$(s) 1 Alanine(c) | 1 | 2 | - | - | - | - | - | - | 1 | - | 7 | - |
| 481 Arginine | Arginine(c) | −$NH_3$(c) MCES | de novo synthesis of cytosolic Arginine | 4 $NH_3$(c) 2 Pyruvate(m) 2 ATP-energy(c) 3 ATP-energy(m) 2 NADPH-redox-potential(m) 3 Proton-gradient(m) | 4 $H_2O$(s) 1 Arginine(c) 1 NADH-redox-potential(c) | 9 | 15 | - | - | - | - | - | - | 1 | - | 8 | - |

Continued on next page

C2. Precursors for macromolecules – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 482 Asparagine | Asparagine(c) | −Histidine(c) MCES | de novo synthesis of cytosolic Asparagine | 0.67 $H_2O$(s) 0.33 $O_2$(s) 0.33 Pyruvate(m) 0.67 Histidine(c) 3 ATP-energy(c) 0.67 NADPH-redox-potential(c) 0.33 NADPH-redox-potential(m) | 0.33 $CO_2$(s) 1 Asparagine(c) 0.67 ATP-energy(m) 0.33 NADH-redox-potential(c) 0.33 NADH-redox-potential(m) 3.67 Proton-gradient(m) 0.67 THF-activated methyl group(c) | 17 | 10 | - | - | - | - | - | - | 3 | - | 10 | - |
| 483 Aspartate | Aspartate(c) | −Histidine(c) MCES | de novo synthesis of cytosolic Aspartate | 0.33 $H_2O$(s) 0.17 $O_2$(s) 1 Pyruvate(m) 0.33 Histidine(c) 0.33 NADPH-redox-potential(c) 0.67 NADPH-redox-potential(m) | 1 Aspartate(c) 0.33 ATP-energy(m) 0.67 NADH-redox-potential(c) 1.33 Proton-gradient(m) 0.33 THF-activated methyl group(c) 0.33 CoA-activated acetyl group(m) | 12 | 11 | - | - | - | - | - | - | 2 | - | 9 | - |
| 484 Glutamate | Glutamate(c) | −$NH_3$(c) MCES | de novo synthesis of cytosolic Glutamate | 1 $NH_3$(c) 1 Pyruvate(m) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 Glutamate(c) 1 NADH-redox-potential(m) | - | 10 | - | - | - | - | - | - | - | - | 4 | - |
| 485 Glycine | Glycine(c) | −$NH_3$(c) MCES | de novo synthesis of cytosolic Glycine | 1 $NH_3$(c) 0.5 Glucose-6P(c) 1 NADH-redox-potential(m) 2 Proton-gradient(m) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 Glycine(c) 0.5 ATP-energy(c) 1 NADH-redox-potential(c) 1 THF-activated methyl group(c) | 14 | 2 | - | - | - | - | - | - | 1 | - | 7 | - |
| 486 Glutamine | Glutamine(c) | −$NH_3$(c) MCES | de novo synthesis of cytosolic Glutamine | 2 $NH_3$(c) 1 Pyruvate(m) 1 ATP-energy(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 1 CoA-activated acetyl group(m) | 1 $H_2O$(s) 1 Glutamine(c) 1 NADH-redox-potential(m) | 2 | 10 | - | - | - | - | - | - | 1 | - | 4 | - |
| 487 Proline | Proline(c) | −Valine(c) MCES | de novo synthesis of cytosolic Proline | 1 $O_2$(s) 1 Valine(c) 1 ATP-energy(m) 1 NADPH-redox-potential(m) | 2 $H_2O$(s) 1 Proline(c) 2 NADH-redox-potential(m) 10 Proton-gradient(m) | - | 16 | - | - | - | - | - | - | 2 | - | 7 | - |
| 488 Serine | Serine(c) | −$NH_3$(c) MCES | de novo synthesis of cytosolic Serine | 0.5 $H_2O$(s) 1 $NH_3$(c) 0.5 Glucose-6P(c) 1 NADH-redox-potential(m) 2 Proton-gradient(m) | 0.5 $P_i$(c) 1 Serine(c) 0.5 ATP-energy(c) 2 NADH-redox-potential(c) | 11 | 2 | - | - | - | - | - | - | 1 | - | 7 | - |
| 489 Tyrosine | Tyrosine(c) | −Phenylalanine(c) MCES | de novo synthesis of cytosolic Tyrosine | 1 $O_2$(s) 1 Phenylalanine(c) 1 NADH-redox-potential(c) | 1 $H_2O$(s) 1 Tyrosine(c) | 3 | - | - | - | - | - | - | - | 2 | - | - | - |
| **C2.4. For lipids** | | | | | | | | | | | | | | | | | |

Continued on next page

C2. Precursors for macromolecules – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 490 Palmitate | Palmitate(c) | MCES | de novo synthesis of cytosolic Palmitate | 7 ATP-energy(c) 14 NADPH-redox-potential(c) 8 CoA-activated acetyl group(c) | 6 $H_2O$(s) 1 Palmitate(c) | 37 | - | - | - | - | - | - | - | 1 | - | - | - |
| 491 Glycerol | Glycerol(c) | MCES | de novo synthesis of cytosolic Glycerol | 0.5 $H_2O$(s) 0.5 Glucose-6P(c) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $P_i$(c) 1 Glycerol(c) | 26 | - | - | - | - | - | - | - | 1 | - | - | - |
| 492 Oleate | Oleate(c) | MCES | de novo synthesis of cytosolic Oleate | 1 $O_2$(s) 10 ATP-energy(c) 1 NADH-redox-potential(c) 16 NADPH-redox-potential(c) 9 CoA-activated acetyl group(c) | 9 $H_2O$(s) 1 Oleate(c) | 47 | - | - | - | - | - | - | - | 2 | - | - | - |
| 493 Stearate | Stearate(c) | MCES | de novo synthesis of cytosolic Stearate | 8 ATP-energy(c) 16 NADPH-redox-potential(c) 9 CoA-activated acetyl group(c) | 7 $H_2O$(s) 1 Stearate(c) | 41 | - | - | - | - | - | - | - | 1 | - | - | - |
| **C2.5. Activated sugars** | | | | | | | | | | | | | | | | | |
| 494 Mannose-1P | Mannose-1P(c) | MCES | de novo synthesis of cytosolic Mannose-1P | 1 Glucose-6P(c) | 1 Mannose-1P(c) | 3 | - | - | - | - | - | - | - | - | - | - | - |
| 495 Mannose-6P | Mannose-6P(c) | MCES | de novo synthesis of cytosolic Mannose-6P | 1 Glucose-6P(c) | 1 Mannose-6P(c) | 2 | - | - | - | - | - | - | - | - | - | - | - |
| 496 Fructose-6P | Fructose-6P(c) | MCES | de novo synthesis of cytosolic Fructose-6P | 1 Glucose-6P(c) | 1 Fructose-6P(c) | 1 | - | - | - | - | - | - | - | - | - | - | - |
| 497 UDP-xylose | UDP-xylose(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic UDP-xylose | 0.5 $O_2$(s) 0.17 $P_i$(c) 1 Aspartate(c) 1 Glutamine(c) 1.83 Glucose-6P(c) 6.17 ATP-energy(c) | 3.17 $H_2O$(s) 1 $CO_2$(s) 1 Glutamate(c) 1 UDP-xylose(c) 2 NADH-redox-potential(c) 6 Proton-gradient(m) | 26 | - | 1 | - | - | - | - | - | 3 | - | 9 | - |
| 498 UDP-glucose | UDP-glucose(c) | MCES −Glutamine(c) +Glutamate(c) −Aspartate(c) | de novo synthesis of cytosolic UDP-glucose | 0.5 $O_2$(s) 0.17 $P_i$(c) 1 Aspartate(c) 1 Glutamine(c) 1.83 Glucose-6P(c) 6.17 ATP-energy(c) | 4.17 $H_2O$(s) 1 Glutamate(c) 1 UDP-glucose(c) 6 Proton-gradient(m) | 24 | - | - | - | - | - | - | - | 2 | - | 6 | - |

Continued on next page

C2. Precursors for macromolecules – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 499 udpgal | UDP-galactose(c) | MCES −Glutamine(c) +Glutamate(c) −Aspartate(c) | de novo synthesis of cytosolic UDP-galactose | 0.5 $O_2$(s) 0.17 $P_i$(c) 1 Aspartate(c) 1 Glutamine(c) 1.83 Glucose-6P(c) 6.17 ATP-energy(c) | 4.17 $H_2O$(s) 1 Glutamate(c) 1 UDP-galactose(c) 6 Proton-gradient(m) | 25 | - | - | - | - | - | - | - | 2 | - | 6 | - |
| 500 udpglcur | UDP-glucuronate(c) | MCES −Glutamine(c) +Glutamate(c) −Aspartate(c) | de novo synthesis of cytosolic UDP-glucuronate | 0.5 $O_2$(s) 0.17 $P_i$(c) 1 Aspartate(c) 1 Glutamine(c) 1.83 Glucose-6P(c) 6.17 ATP-energy(c) | 3.17 $H_2O$(s) 1 Glutamate(c) 1 UDP-glucuronate(c) 2 NADH-redox-potential(c) 6 Proton-gradient(m) | 26 | - | - | - | - | - | - | - | 2 | - | 6 | - |
| 501 GDP-L-fucose | GDP-L-fucose(c) | MCES −Glutamine(c) +Glutamate(c) −Aspartate(c) | de novo synthesis of cytosolic GDP-L-fucose | 2 Aspartate(c) 3 Glutamine(c) 2.33 Glucose-6P(c) 9.67 ATP-energy(c) 1 THF-activated methyl group(c) | 1.67 $H_2O$(s) 0.33 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 3 Glutamate(c) 1 GDP-L-fucose(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) | 48 | - | - | - | - | - | - | - | 2 | - | - | - |
| 502 GDP-mannose | GDP-mannose(c) | MCES −Glutamine(c) +Glutamate(c) −Aspartate(c) | de novo synthesis of cytosolic GDP-mannose | 2 Aspartate(c) 3 Glutamine(c) 2.33 Glucose-6P(c) 9.67 ATP-energy(c) 1 THF-activated methyl group(c) | 0.67 $H_2O$(s) 0.33 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 3 Glutamate(c) 1 GDP-mannose(c) 2 NADH-redox-potential(c) 5 NADPH-redox-potential(c) | 46 | - | - | - | - | - | - | - | 2 | - | - | - |
| **C2.6. Other** | | | | | | | | | | | | | | | | | |
| 503 IMP | IMP(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic IMP | 2 Aspartate(c) 2 Glutamine(c) 1.33 Glucose-6P(c) 5.67 ATP-energy(c) 1 THF-activated methyl group(c) | 0.67 $H_2O$(s) 0.33 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(c) 1 IMP(c) 1 NADH-redox-potential(c) 5 NADPH-redox-potential(c) | 39 | - | - | - | - | - | - | - | 2 | - | - | - |
| 504 XMP | Xanthosine-5P(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic Xanthosine-5P | 0.33 $H_2O$(s) 2 Aspartate(c) 2 Glutamine(c) 1.33 Glucose-6P(c) 5.67 ATP-energy(c) 1 THF-activated methyl group(c) | 0.33 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(c) 1 Xanthosine-5P(c) 2 NADH-redox-potential(c) 5 NADPH-redox-potential(c) | 40 | - | - | - | - | - | - | - | 2 | - | - | - |
| 505 Uracil | Uracil(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic Uracil | 0.5 $O_2$(s) 1 Aspartate(c) 1 Glutamine(c) 3 ATP-energy(c) | 2 $H_2O$(s) 1 Glutamate(c) 1 Uracil(c) 6 Proton-gradient(m) | 14 | - | - | - | - | - | - | - | 2 | - | 6 | - |
| 506 Uridine | Uridine(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic Uridine | 0.5 $O_2$(s) 1 Aspartate(c) 1 Glutamine(c) 0.83 Glucose-6P(c) 3.17 ATP-energy(c) | 2.17 $H_2O$(s) 0.83 $P_i$(c) 1 Glutamate(c) 1 Uridine(c) 6 Proton-gradient(m) | 21 | - | - | - | - | - | - | - | 2 | - | 6 | - |

Continued on next page

C2. Precursors for macromolecules – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 507 Cytidine | Cytidine(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) $-NH_3$(c) MCES | de novo synthesis of cytosolic Cytidine | 0.5 $O_2$(s) 1 Aspartate(c) 2 Glutamine(c) 0.83 Glucose-6P(c) 5.17 ATP-energy(c) | 2.17 $H_2O$(s) 0.83 $P_i$(c) 2 Glutamate(c) 1 Cytidine(c) 6 Proton-gradient(m) | 26 | - | - | - | - | - | - | - | 2 | - | 6 | - |
| 508 Xanthine | Xanthine(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic Xanthine | 1.5 $H_2O$(s) 2 Aspartate(c) 2 Glutamine(c) 0.5 Glucose-6P(c) 5.5 ATP-energy(c) 1 THF-activated methyl group(c) | 0.5 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(c) 1 Xanthine(c) 3 NADH-redox-potential(c) 4 NADPH-redox-potential(c) | 38 | - | - | - | - | - | - | - | 2 | - | - | - |
| 509 Guanine | Guanine(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic Guanine | 1.5 $H_2O$(s) 2 Aspartate(c) 3 Glutamine(c) 0.5 Glucose-6P(c) 7.5 ATP-energy(c) 1 THF-activated methyl group(c) | 0.5 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 3 Glutamate(c) 1 Guanine(c) 2 NADH-redox-potential(c) 5 NADPH-redox-potential(c) | 39 | - | - | - | - | - | - | - | 2 | - | - | - |
| 510 Adenosine | Adenosine(c) | −Glutamine(c) +Glutamate(c) −Aspartate(c) MCES | de novo synthesis of cytosolic Guanine | 0.33 $H_2O$(s) 3 Aspartate(c) 2 Glutamine(c) 1.33 Glucose-6P(c) 5.67 ATP-energy(c) 1 THF-activated methyl group(c) | 1.33 $P_i$(c) 2 $CO_2$(s) 3 Pyruvate(c) 2 Glutamate(c) 1 Adenosine(c) 1 NADH-redox-potential(c) 6 NADPH-redox-potential(c) | 43 | - | - | - | - | - | - | - | 2 | - | - | - |
| 511 UDP-N-acetylgalactosamine | UDP-N-acetyl-D-galactosamine(c) | MCES AAA | de novo synthesis of cytosolic UDP-N-acetyl-D-galactosamine | 0.33 $O_2$(s) 0.17 $P_i$(c) 1 Glutamine(s) 1.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 6.17 ATP-energy(c) 1 CoA-activated acetyl group(c) | 3.17 $H_2O$(s) 1.33 Glutamate(s) 1 UDP-N-acetyl-D-galactosamine(c) 0.33 NADH-redox-potential(m) 1 Proton-gradient(c) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 29 | 4 | - | - | - | - | - | - | 8 | - | 6 | - |
| 512 N-acglucam | N-Acetylglucosamine(c) | MCES AAA | de novo synthesis of cytosolic N-Acetylglucosamine | 1 Serine(s) 1 Glucose-6P(c) 1 ATP-energy(c) 1 CoA-activated acetyl group(c) | 1 $P_i$(c) 1 Pyruvate(c) 1 N-Acetylglucosamine(c) | 12 | - | - | - | - | - | - | - | 1 | - | - | - |
| 513 CMP-N-acetylneuraminate | CMP-N-acetylneuraminate(n) | MCES −CMP(c) +Glutamate −Glutamine =Asparagine =Proline =Cystine $=H_2S$ $=NH_3$ | Synthesis of CMP-N-acetylneuraminate in nucleus | 1 Pyruvate(c) 1 CMP(c) 1 Glutamine(s) 1 Glucose-6P(c) 5 ATP-energy(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 1 $P_i$(c) 1 Glutamate(s) 1 CMP-N-acetylneuraminate(n) 1 NADH-redox-potential(c) | 21 | - | - | - | - | 1 | - | - | 2 | - | 3 | - |



## 4.3 C3. Constituents of cellular structures

Table 14: C3. Constituents of cellular structures

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| **C3.1. Lipids** | | | | | | | | | | | | | | | | | | |
| 514 PC | PC-VLDL-pool(c) | MCES ALFA | de novo synthesis of cytosolic PC-VLDL-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Choline(c) 0.17 Arachidonate(c) 0.7 Palmitate(c) 0.27 Oleate(c) 0.3 Stearate(c) 0.55 Linoleate(c) 7.5 ATP-energy(c) 1 NADH-redox-potential(c) | 3.5 $H_2O$(s) 1 PC-VLDL-pool(c) | 28 | - | - | - | - | - | - | - | 1 | - | - | - | |
| 515 PE | PE-VLDL-pool(c) | MCES ALFA | de novo synthesis of cytosolic PE-VLDL-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 0.6 Arachidonate(c) 0.34 Palmitate(c) 0.17 Oleate(c) 0.54 Stearate(c) 0.36 Linoleate(c) 7.5 ATP-energy(c) 1 NADH-redox-potential(c) | 3.5 $H_2O$(s) 1 PE-VLDL-pool(c) | 28 | - | - | - | - | - | - | - | 1 | - | - | - | |
| 516 PS | PS-VLDL-pool(c) | MCES ALFA | de novo synthesis of cytosolic PS-VLDL-pool | 0.5 $P_i$(c) 1 Pyruvate(m) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 0.53 Arachidonate(c) 0.09 Palmitate(c) 0.09 Oleate(c) 1.25 Stearate(c) 0.05 Linoleate(c) 7.5 ATP-energy(c) 1 NADH-redox-potential(c) | 3.5 $H_2O$(s) 1 PS-VLDL-pool(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 29 | 3 | - | - | - | - | - | - | 1 | - | 1 | - | |
| 517 PI | PI-pool(c) | MCES ALFA | de novo synthesis of cytosolic PI-pool | 1.5 Glucose-6P(c) 0.51 Arachidonate(c) 0.16 Palmitate(c) 0.32 Oleate(c) 0.85 Stearate(c) 0.16 Linoleate(c) 6.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 0.5 $P_i$(c) 1 PI-pool(c) | 28 | - | - | - | - | - | - | - | 1 | - | - | - | |
| 518 CL | CL-pool(m) | MCES ALFA | de novo synthesis of mitochondrial CL-pool | 2 Glucose-6P(c) 0.17 Palmitate(c) 0.56 Oleate(c) 0.08 Stearate(c) 3 Linoleate(c) 0.19 Palmitolate(c) 10 ATP-energy(c) 4 ATP-energy(m) 4 NADH-redox-potential(c) 1 Proton-gradient(m) | 6 $H_2O$(s) 1 $P_i$(c) 1 CL-pool(m) | 15 | 10 | - | - | - | - | - | - | 1 | - | 5 | - | |

Continued on next page

C3. Constituents of cellular structures – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 519 LacCer | LacCer-pool(r) | MCES ALFA | de novo synthesis of LacCer-pool in ER/Golgi | 2.5 Glucose-6P(c) 1 Ethanolamine(c) 0.02 Arachidonate(c) 0.91 Palmitate(c) 0.24 Oleate(c) 0.03 gamma-Linolenate(c) 0.8 Palmitolate(c) 9.5 ATP-energy(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 2 Proton-gradient(m) | 1.53 $H_2O$(s) 2.5 $P_i$(c) 1 $CO_2$(s) 3 NADH-redox-potential(c) 1 LacCer-pool(r) 1 CoA-activated acetyl group(c) | 39 | 2 | 2 | - | - | - | - | - | 2 | - | 11 | - |
| 520 SM | SM-pool(c) | MCES ALFA | de novo synthesis of cytosolic SM-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Choline(c) 1 Ethanolamine(c) 0.02 Arachidonate(c) 0.91 Palmitate(c) 0.24 Oleate(c) 0.03 gamma-Linolenate(c) 0.8 Palmitolate(c) 9.5 ATP-energy(c) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 3.53 $H_2O$(s) 1 $CO_2$(s) 1 SM-pool(c) 3 NADH-redox-potential(c) 1 CoA-activated acetyl group(c) | 37 | 2 | 1 | - | - | - | - | - | 2 | - | 11 | - |
| 521 Ceramide | Ceramide-pool(c) | MCES ALFA | de novo synthesis of cytosolic Ceramide-pool | 0.5 Glucose-6P(c) 1 Ethanolamine(c) 0.02 Arachidonate(c) 0.91 Palmitate(c) 0.24 Oleate(c) 0.03 gamma-Linolenate(c) 0.8 Palmitolate(c) 6.5 ATP-energy(c) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 1.53 $H_2O$(s) 0.5 $P_i$(c) 1 $CO_2$(s) 1 Ceramide-pool(c) 3 NADH-redox-potential(c) 1 CoA-activated acetyl group(c) | 33 | 2 | - | - | - | - | - | - | 2 | - | 7 | - |
| 522 Triacylglycerol | Triacylglycerol-VLDL-pool(r) | MCES ALFA | de novo synthesis of Triacylglycerol-VLDL-pool in ER/Golgi | 0.5 Glucose-6P(c) 0.09 Arachidonate(c) 0.92 Palmitate(c) 1.1 Oleate(c) 0.2 Stearate(c) 0.69 Linoleate(c) 6.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 0.5 $P_i$(c) 1 Triacylglycerol-VLDL-pool(r) | 25 | - | - | - | - | - | - | - | 1 | - | 1 | - |
| 523 Cholesterol | Cholesterol(r) | MCES | de novo synthesis of Cholesterol in ER/Golgi | 8 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 11 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 16 | - | - | - | - | - | 3 | - | 5 | - |

## 4.4 C4. Other building blocks

Table 15: C4. Other building blocks

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 524 gdpddman | GDP-4-dehydro-6-deoxy-D-mannose(c) | MCES −Glutamine(c) +Glutamate(c) −Aspartate(c) | de novo synthesis of cytosolic GDP-4-dehydro-6-deoxy-D-mannose | 2 Aspartate(c) 3 Glutamine(c) 2.33 Glucose-6P(c) 9.67 ATP-energy(c) 1 THF-activated methyl group(c) | 1.67 $H_2O$(s) 0.33 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 3 Glutamate(c) 1 GDP-4-dehydro-6-deoxy-D-mannose(c) 2 NADH-redox-potential(c) 5 NADPH-redox-potential(c) | 47 | - | - | - | - | - | - | - | 2 | - | - | - |
| 525 beta-Alanine | beta-Alanine(c) | MCES −Glutamine(c) +Glutamate(c) | de novo synthesis of cytosolic beta-Alanine | 0.33 $H_2O$(s) 0.17 $O_2$(s) 0.67 Pyruvate(m) 0.67 Glutamine(c) 1.33 NADPH-redox-potential(m) | 0.67 $CO_2$(s) 0.33 Glutamate(c) 1 beta-Alanine(c) 0.67 NADH-redox-potential(c) 0.67 NADH-redox-potential(m) 1.67 Proton-gradient(m) | 6 | 13 | - | - | - | - | - | - | 3 | - | 10 | - |
| 526 Putrescine | Putrescine(c) | MCES −Glutamine(c) +Glutamate(c) | de novo synthesis of cytosolic Putrescine | 1 Glutamine(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 2 Proton-gradient(m) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Putrescine(c) | 1 | 6 | - | - | - | - | - | - | 2 | - | 4 | - |
| 527 Spermidine | Spermidine | MCES +Methylthioribose-1P(c) −Glutamine(c) +Glutamate(c) −Methionine(c) | test that cytosolic Spermidine can be produced from the minimal exchange set while the cytosolic dump of Methylthioribose-1P is allowed | 0.17 $P_i$(c) 1 Glutamine(c) 1 Methionine(c) 0.83 Glucose-6P(c) 4.17 ATP-energy(c) 1 NADH-redox-potential(m) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) | 2.17 $H_2O$(s) 2 $CO_2$(s) 1 Spermidine(s) 1 Methylthioribose-1P(c) | 19 | 6 | - | - | - | - | - | - | 3 | - | 4 | - |

Continued on next page

C4. Other building blocks – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 528 Spermine | Spermine | MCES +Methylthioribose-1P(c) −Glutamine(c) +Glutamate(c) −Methionine(c) | test that cytosolic Spermine can be produced from the minimal exchange set while the cytosolic dump of Methylthioribose-1P is allowed | 0.33 $P_i$(c) 1 Glutamine(c) 2 Methionine(c) 1.67 Glucose-6P(c) 8.33 ATP-energy(c) 2 NADH-redox-potential(m) 1 Proton-gradient(m) | 3.33 $H_2O$(s) 3 $CO_2$(s) 1 Spermine(s) 2 Methylthioribose-1P(c) | 20 | 5 | - | - | - | - | - | - | 3 | - | 4 | - | |
| 529 Methylthioribose-1P | Methylthioribose-1P(c) | +Spermidine MCES −Glutamine(c) +Glutamate(c) −Methionine(c) | test that cytosolic Methylthioribose-1P can be produced from the minimal exchange set while the cytosolic dump of Spermidine is allowed | 0.17 $P_i$(c) 1 Methionine(c) 0.83 Glucose-6P(c) 4.17 ATP-energy(c) | 1.17 $H_2O$(s) 1 $CO_2$(s) 1 Adenosylmethioninamine-potential(c) 1 Methylthioribose-1P(c) | 18 | - | - | - | - | - | - | - | 2 | - | - | - | |

## 4.5 C5. Comprehensive list

Table 16: C5. Comprehensive list

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 530 (2E)-Decenoyl-ACP | (2E)-Decenoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (2E)-Decenoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 628 ATP-energy(c) 7 NADPH-redox-potential(c) 3 Proton-gradient(c) 5 CoA-activated acetyl group(c) | 7 $H_2O$(s) 1 $CO_2$(s) 1 (2E)-Decenoyl-ACP(c) 66 Na-gradient(c) | 34 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 531 (2E)-Decenoyl-CoA | (2E)-Decenoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (2E)-Decenoyl-CoA | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (2E)-Decenoyl-CoA(m) 2 NADH-redox-potential(c) 4 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 6 Proton-gradient(m) 3 Na-gradient(c) 4 CoA-activated acetyl group(m) | 44 | 19 | - | - | - | - | - | - | 12 | - | 7 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 532 (2E)-Dodecenoyl-ACP | (2E)-Dodecenoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (2E)-Dodecenoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 629 ATP-energy(c) 9 NADPH-redox-potential(c) 3 Proton-gradient(c) 6 CoA-activated acetyl group(c) | 8 $H_2O$(s) 1 $CO_2$(s) 1 (2E)-Dodecenoyl-ACP(c) 66 Na-gradient(c) | 38 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 533 (2E)-Dodecenoyl-CoA | (2E)-Dodecenoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (2E)-Dodecenoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (2E)-Dodecenoyl-CoA(m) 2 NADH-redox-potential(c) 3 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 3 Na-gradient(c) 3 CoA-activated acetyl group(m) | 44 | 15 | - | - | - | - | - | - | 11 | - | 3 | - |
| 534 (2E)-Hexadecenoyl-ACP | (2E)-Hexadecenoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (2E)-Hexadecenoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 631 ATP-energy(c) 13 NADPH-redox-potential(c) 3 Proton-gradient(c) 8 CoA-activated acetyl group(c) | 10 $H_2O$(s) 1 $CO_2$(s) 1 (2E)-Hexadecenoyl-ACP(c) 66 Na-gradient(c) | 46 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 535 (2E)-Hexadecenoyl-CoA | (2E)-Hexadecenoyl-CoA(c) | PIPES MCES | synthesis of cytosolic (2E)-Hexadecenoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (2E)-Hexadecenoyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 11 | - | - | - |
| 536 (2E)-Hexenoyl-ACP | (2E)-Hexenoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (2E)-Hexenoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 626 ATP-energy(c) 3 NADPH-redox-potential(c) 3 Proton-gradient(c) 3 CoA-activated acetyl group(c) | 5 $H_2O$(s) 1 $CO_2$(s) 1 (2E)-Hexenoyl-ACP(c) 66 Na-gradient(c) | 26 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 537 (2E)-Hexenoyl-CoA | (2E)-Hexenoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (2E)-Hexenoyl-CoA | 1.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (2E)-Hexenoyl-CoA(m) 2 NADH-redox-potential(c) 6 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 2 Proton-gradient(c) 18 Proton-gradient(m) 5 Na-gradient(c) 6 CoA-activated acetyl group(m) | 44 | 27 | - | - | - | - | - | - | 12 | - | 7 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 538 (2E)-Octadecenoyl-ACP | (2E)-Octadecenoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (2E)-Octadecenoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 632 ATP-energy(c) 15 NADPH-redox-potential(c) 3 Proton-gradient(c) 9 CoA-activated acetyl group(c) | 11 $H_2O$(s) 1 $CO_2$(s) 1 (2E)-Octadecenoyl-ACP(c) 66 Na-gradient(c) | 50 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 539 (2E)-Octenoyl-ACP | (2E)-Octenoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (2E)-Octenoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 627 ATP-energy(c) 5 NADPH-redox-potential(c) 3 Proton-gradient(c) 4 CoA-activated acetyl group(c) | 6 $H_2O$(s) 1 $CO_2$(s) 1 (2E)-Octenoyl-ACP(c) 66 Na-gradient(c) | 30 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 540 (2E)-Octenoyl-CoA | (2E)-Octenoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (2E)-Octenoyl-CoA | 1 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (2E)-Octenoyl-CoA(m) 2 NADH-redox-potential(c) 5 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 2 Proton-gradient(c) 12 Proton-gradient(m) 5 Na-gradient(c) 5 CoA-activated acetyl group(m) | 44 | 23 | - | - | - | - | - | - | 12 | - | 7 | - |
| 541 (2E)-Tetradecenoyl-ACP | (2E)-Tetradecenoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (2E)-Tetradecenoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 630 ATP-energy(c) 11 NADPH-redox-potential(c) 3 Proton-gradient(c) 7 CoA-activated acetyl group(c) | 9 $H_2O$(s) 1 $CO_2$(s) 1 (2E)-Tetradecenoyl-ACP(c) 66 Na-gradient(c) | 42 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 542 (2E)-Tetradecenoyl-CoA | (2E)-Tetradecenoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (2E)-Tetradecenoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 0.17 Palmitate(s) 0.5 Cystine(s) 1 Pantothenate(s) 0.83 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 4.5 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2.33 Glutamate(s) 1 (2E)-Tetradecenoyl-CoA(m) 2.83 NADH-redox-potential(c) 1.33 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 Proton-gradient(c) 10 Proton-gradient(m) 5.33 Na-gradient(c) 1 CoA-activated acetyl group(m) | 47 | 11 | - | - | - | - | - | - | 13 | - | 7 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 543 (3Z)-Dodecenoyl-CoA | (3Z)-Dodecenoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (3Z)-Dodecenoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (3Z)-Dodecenoyl-CoA(m) 2 NADH-redox-potential(c) 3 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 3 Na-gradient(c) 3 CoA-activated acetyl group(m) | 44 | 14 | - | - | - | - | - | - | 11 | - | 3 | - |
| 544 (R)-3-Hydroxybutanoyl-ACP | (R)-3-Hydroxybutanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (R)-3-Hydroxybutanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 625 ATP-energy(c) 1 NADPH-redox-potential(c) 2 CoA-activated acetyl group(c) | 3 $H_2O$(s) 1 $CO_2$(s) 1 (R)-3-Hydroxybutanoyl-ACP(c) 2 Proton-gradient(c) 82 Na-gradient(c) | 21 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 545 (R)-3-Hydroxydecanoyl-ACP | (R)-3-Hydroxydecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (R)-3-Hydroxydecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 628 ATP-energy(c) 7 NADPH-redox-potential(c) 3 Proton-gradient(c) 5 CoA-activated acetyl group(c) | 6 $H_2O$(s) 1 $CO_2$(s) 1 (R)-3-Hydroxydecanoyl-ACP(c) 66 Na-gradient(c) | 33 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 546 (R)-3-Hydroxyoctanoyl-ACP | (R)-3-Hydroxyoctanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (R)-3-Hydroxyoctanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 627 ATP-energy(c) 5 NADPH-redox-potential(c) 3 Proton-gradient(c) 4 CoA-activated acetyl group(c) | 5 $H_2O$(s) 1 $CO_2$(s) 1 (R)-3-Hydroxyoctanoyl-ACP(c) 66 Na-gradient(c) | 29 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 547 (R)-3-Hydroxypalmitoyl-ACP | (R)-3-Hydroxypalmitoyl-ACP(c) | PIPES MCES | synthesis of cytosolic (R)-3-Hydroxypalmitoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 631 ATP-energy(c) 13 NADPH-redox-potential(c) 3 Proton-gradient(c) 8 CoA-activated acetyl group(c) | 9 $H_2O$(s) 1 $CO_2$(s) 1 (R)-3-Hydroxypalmitoyl-ACP(c) 66 Na-gradient(c) | 45 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 548 (R)-4-Phosphopantothenoyl-cysteine | (R)-4-Phosphopantothenoyl-cysteine(c) | PIPES MCES | synthesis of cytosolic (R)-4-Phosphopantothenoyl-cysteine | 1 $P_i$(c) 1 Cysteine(s) 1 Pantothenate(s) 3 ATP-energy(c) | 2 $H_2O$(s) 1 (R)-4-Phosphopantothenoyl-cysteine(c) 1 Na-gradient(c) | 6 | - | - | - | - | - | - | - | 4 | - | - | - |
| 549 (R)-5-Diphosphomevalonate | (R)-5-Diphosphomevalonate(p) | PIPES MCES | synthesis of peroxysomal (R)-5-Diphosphomevalonate | 2 $P_i$(c) 2 ATP-energy(c) 2 NADPH-redox-potential(c) 3 CoA-activated acetyl group(c) | 1 $H_2O$(s) 1 (R)-5-Diphosphomevalonate(p) | 6 | - | - | 2 | - | - | - | - | 1 | - | 2 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 550 (R)-5-Phosphomevalonate | (R)-5-Phosphomevalonate(p) | PIPES MCES | synthesis of peroxysomal (R)-5-Phosphomevalonate | 1 $P_i$(c) 1 ATP-energy(c) 2 NADPH-redox-potential(c) 3 CoA-activated acetyl group(c) | 1 (R)-5-Phosphomevalonate(p) | 6 | - | - | 1 | - | - | - | - | - | - | 2 | - |
| 551 (R)-Methylmalonyl-CoA | (R)-Methylmalonyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (R)-Methylmalonyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 1 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 Proton-gradient(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 1 Pyruvate(c) 1 Glutamate(s) 1 (R)-Methylmalonyl-CoA(m) 3 NADH-redox-potential(c) 1 NADH-redox-potential(m) 2.5 NADPH-redox-potential(c) 4 Na-gradient(c) | 44 | 3 | - | - | - | - | - | - | 10 | - | 5 | - |
| 552 (R)-Mevalonate | (R)-Mevalonate(c) | PIPES MCES | synthesis of cytosolic (R)-Mevalonate | 1 $H_2O$(s) 2 NADPH-redox-potential(c) 3 CoA-activated acetyl group(c) | 1 (R)-Mevalonate(c) | 5 | - | - | - | - | - | - | - | 1 | - | - | - |
| 553 (S)-3-Hydroxy-2-methylbutyryl-CoA | (S)-3-Hydroxy-2-methylbutyryl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-3-Hydroxy-2-methylbutyryl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 1.5 Aspartate(s) 0.5 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Asparagine(s) 1 Threonine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.7 ATP-energy(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 6.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 (S)-3-Hydroxy-2-methylbutyryl-CoA(m) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3.5 Na-gradient(c) | 45 | 4 | - | - | - | - | - | - | 10 | - | 4 | - |
| 554 (S)-3-Hydroxybutyryl-CoA | (S)-3-Hydroxybutyryl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-3-Hydroxybutyryl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 NADH-redox-potential(m) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (S)-3-Hydroxybutyryl-CoA(m) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 42 | 4 | - | - | - | - | - | - | 10 | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 555 (S)-3-Hydroxydodecanoyl-CoA | (S)-3-Hydroxydodecanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-3-Hydroxydodecanoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (S)-3-Hydroxydodecanoyl-CoA(m) 2 NADH-redox-potential(c) 3 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 3 Na-gradient(c) 3 CoA-activated acetyl group(m) | 44 | 16 | - | - | - | - | - | - | 11 | - | 3 | - |
| 556 (S)-3-Hydroxyhexadecanoyl-CoA | (S)-3-Hydroxyhexadecanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-3-Hydroxyhexadecanoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Palmitate(s) 0.5 Cystine(s) 1 Pantothenate(s) 0.5 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (S)-3-Hydroxyhexadecanoyl-CoA(m) 0.5 NADH-redox-potential(c) 5.5 NADPH-redox-potential(c) 6 Proton-gradient(m) 3 Na-gradient(c) | 47 | 3 | - | - | - | - | - | - | 12 | - | 6 | - |
| 557 (S)-3-Hydroxytetradecanoyl-CoA | (S)-3-Hydroxytetradecanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-3-Hydroxytetradecanoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 0.5 Aspartate(s) 0.5 Glutamine(s) 0.83 Glucose-6P(c) 1.5 Asparagine(s) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 14.7 ATP-energy(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 (S)-3-Hydroxytetradecanoyl-CoA(m) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 5.5 NADPH-redox-potential(c) 12 Proton-gradient(m) 2.5 Na-gradient(c) 1 CoA-activated acetyl group(m) | 48 | 9 | - | - | - | - | - | - | 10 | - | 6 | - |
| 558 (S)-3-hydroxyoleyleoyl-CoA | (S)-3-hydroxyoleyleoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-3-hydroxyoleyleoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 NADH-redox-potential(m) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 (S)-3-hydroxyoleyleoyl-CoA(m) 3 Na-gradient(c) | 43 | 4 | - | - | - | - | - | - | 11 | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 559 (S)-3-hydroxypalmitoleoyl-CoA | (S)-3-hydroxypalmitoleoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-3-hydroxypalmitoleoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 FADH-redox-potential(c) 1 (S)-3-hydroxypalmitoleoyl-CoA(m) 3 Na-gradient(c) | 44 | 2 | - | - | - | - | - | - | 11 | - | 3 | - |
| 560 (S)-Dihydroorotate | (S)-Dihydroorotate(c) | PIPES MCES | synthesis of cytosolic (S)-Dihydroorotate | 0.5 Pyruvate(m) 1 Asparagine(s) 3 ATP-energy(c) 0.5 THF-activated methyl group(c) | 1 (S)-Dihydroorotate(c) 0.5 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 0.5 CoA-activated acetyl group(m) | 15 | 3 | - | - | - | - | - | - | 1 | - | 1 | - |
| 561 (S)-Hydroxydecanoyl-CoA | (S)-Hydroxydecanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-Hydroxydecanoyl-CoA | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (S)-Hydroxydecanoyl-CoA(m) 2 NADH-redox-potential(c) 4 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 6 Proton-gradient(m) 3 Na-gradient(c) 4 CoA-activated acetyl group(m) | 44 | 20 | - | - | - | - | - | - | 12 | - | 7 | - |
| 562 (S)-Hydroxyhexanoyl-CoA | (S)-Hydroxyhexanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-Hydroxyhexanoyl-CoA | 1.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 0.5 Aspartate(s) 0.5 Glutamine(s) 0.83 Glucose-6P(c) 1.5 Asparagine(s) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 14.7 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 (S)-Hydroxyhexanoyl-CoA(m) 2 NADH-redox-potential(c) 6 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 0.5 Proton-gradient(c) 18 Proton-gradient(m) 2 Na-gradient(c) 6 CoA-activated acetyl group(m) | 46 | 28 | - | - | - | - | - | - | 12 | - | 7 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | | Definition | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 563 | (S)-Hydroxyoctanoyl-CoA | (S)-Hydroxyoctanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial (S)-Hydroxyoctanoyl-CoA | 1 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 (S)-Hydroxyoctanoyl-CoA(m) 2 NADH-redox-potential(c) 5 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 12 Proton-gradient(m) 3 Na-gradient(c) 5 CoA-activated acetyl group(m) | 44 | 24 | - | - | - | - | - | - | 11 | - | 7 | - | |
| 564 | 1,2-Diacylglycerol-Bile-PC-pool | 1,2-Diacylglycerol-Bile-PC-pool(c) | PIPES MCES | synthesis of cytosolic 1,2-Diacylglycerol-Bile-PC-pool | 0.5 Glucose-6P(c) 0.11 Arachidonate(s) 0.83 Palmitate(s) 0.24 Oleate(s) 0.11 Stearate(s) 0.66 Linoleate(s) 0.05 Palmitolate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 1,2-Diacylglycerol-Bile-PC-pool(c) | 25 | - | - | - | - | - | - | - | 7 | - | - | - | |
| 565 | 1,2-Diacylglycerol-VLDL-PC-pool | 1,2-Diacylglycerol-VLDL-PC-pool(c) | PIPES MCES | synthesis of cytosolic 1,2-Diacylglycerol-VLDL-PC-pool | 0.5 Glucose-6P(c) 0.17 Arachidonate(s) 0.7 Palmitate(s) 0.27 Oleate(s) 0.3 Stearate(s) 0.55 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 1,2-Diacylglycerol-VLDL-PC-pool(c) | 23 | - | - | - | - | - | - | - | 6 | - | - | - | |
| 566 | 1,2-Diacylglycerol-VLDL-PE-pool | 1,2-Diacylglycerol-VLDL-PE-pool(c) | PIPES MCES | synthesis of cytosolic 1,2-Diacylglycerol-VLDL-PE-pool | 0.5 Glucose-6P(c) 0.6 Arachidonate(s) 0.34 Palmitate(s) 0.17 Oleate(s) 0.54 Stearate(s) 0.36 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 1,2-Diacylglycerol-VLDL-PE-pool(c) | 23 | - | - | - | - | - | - | - | 6 | - | - | - | |
| 567 | 1,2-Diacylglycerol-VLDL-PI-pool | 1,2-Diacylglycerol-VLDL-PI-pool(c) | PIPES MCES | synthesis of cytosolic 1,2-Diacylglycerol-VLDL-PI-pool | 0.5 Glucose-6P(c) 0.51 Arachidonate(s) 0.16 Palmitate(s) 0.32 Oleate(s) 0.85 Stearate(s) 0.16 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 1,2-Diacylglycerol-VLDL-PI-pool(c) | 23 | - | - | - | - | - | - | - | 6 | - | - | - | |
| 568 | 1,2-Diacylglycerol-VLDL-PS-pool | 1,2-Diacylglycerol-VLDL-PS-pool(c) | PIPES MCES | synthesis of cytosolic 1,2-Diacylglycerol-VLDL-PS-pool | 0.5 Glucose-6P(c) 0.53 Arachidonate(s) 0.09 Palmitate(s) 0.09 Oleate(s) 1.25 Stearate(s) 0.05 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 1,2-Diacylglycerol-VLDL-PS-pool(c) | 23 | - | - | - | - | - | - | - | 6 | - | - | - | |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 569 1,2-Diacylglycerol-VLDL-SM-pool | 1,2-Diacylglycerol-VLDL-SM-pool(c) | PIPES MCES | synthesis of cytosolic 1,2-Diacylglycerol-VLDL-SM-pool | 0.5 Glucose-6P(c) 0.03 Arachidonate(s) 1.42 Palmitate(s) 0.15 Oleate(s) 0.34 Stearate(s) 0.06 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 1,2-Diacylglycerol-VLDL-SM-pool(c) | 23 | - | - | - | - | - | - | - | 6 | - | - | - |
| 570 1,2-Diacylglycerol-VLDL-TG-pool | 1,2-Diacylglycerol-VLDL-TG-pool(c) | PIPES MCES | synthesis of cytosolic 1,2-Diacylglycerol-VLDL-TG-pool | 0.5 Glucose-6P(c) 0.06 Arachidonate(s) 0.83 Palmitate(s) 0.6 Oleate(s) 0.13 Stearate(s) 0.39 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 1,2-Diacylglycerol-VLDL-TG-pool(c) | 23 | - | - | - | - | - | - | - | 6 | - | - | - |
| 571 1,3DPG | 1,3DPG(c) | PIPES MCES | synthesis of cytosolic 1,3DPG | 1.5 $P_i$(c) 0.5 Glucose-6P(c) 0.5 ATP-energy(c) | 0.5 $H_2O$(s) 1 1,3DPG(c) 1 NADH-redox-potential(c) | 7 | - | - | - | - | - | - | - | 1 | - | - | - |
| 572 1-Acylglycerol-3P-Bile-PC-pool | 1-Acylglycerol-3P-Bile-PC-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-Bile-PC-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.06 Arachidonate(s) 0.41 Palmitate(s) 0.12 Oleate(s) 0.05 Stearate(s) 0.33 Linoleate(s) 0.03 Palmitolate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-Bile-PC-pool(c) | 22 | - | - | - | - | - | - | - | 7 | - | - | - |
| 573 1-Acylglycerol-3P-CL-pool | 1-Acylglycerol-3P-CL-pool(m) | PIPES MCES | synthesis of mitochondrial 1-Acylglycerol-3P-CL-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.04 Palmitate(s) 0.14 Oleate(s) 0.02 Stearate(s) 0.75 Linoleate(s) 0.05 Palmitolate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) 1 Proton-gradient(m) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-CL-pool(m) | 15 | 1 | - | - | - | - | - | - | 6 | - | 5 | - |
| 574 1-Acylglycerol-3P-VLDL-PC-pool | 1-Acylglycerol-3P-VLDL-PC-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-VLDL-PC-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.08 Arachidonate(s) 0.35 Palmitate(s) 0.14 Oleate(s) 0.15 Stearate(s) 0.27 Linoleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-VLDL-PC-pool(c) | 20 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 575 1-Acylglycerol-3P-VLDL-PE-pool | 1-Acylglycerol-3P-VLDL-PE-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-VLDL-PE-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.3 Arachidonate(s) 0.17 Palmitate(s) 0.08 Oleate(s) 0.27 Stearate(s) 0.18 Linoleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-VLDL-PE-pool(c) | 20 | - | - | - | - | - | - | - | 6 | - | - | - |
| 576 1-Acylglycerol-3P-VLDL-PI-pool | 1-Acylglycerol-3P-VLDL-PI-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-VLDL-PI-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.25 Arachidonate(s) 0.08 Palmitate(s) 0.16 Oleate(s) 0.43 Stearate(s) 0.08 Linoleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-VLDL-PI-pool(c) | 20 | - | - | - | - | - | - | - | 6 | - | - | - |
| 577 1-Acylglycerol-3P-VLDL-PS-pool | 1-Acylglycerol-3P-VLDL-PS-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-VLDL-PS-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.27 Arachidonate(s) 0.04 Palmitate(s) 0.04 Oleate(s) 0.62 Stearate(s) 0.02 Linoleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-VLDL-PS-pool(c) | 20 | - | - | - | - | - | - | - | 6 | - | - | - |
| 578 1-Acylglycerol-3P-VLDL-SM-pool | 1-Acylglycerol-3P-VLDL-SM-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-VLDL-SM-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.02 Arachidonate(s) 0.71 Palmitate(s) 0.07 Oleate(s) 0.17 Stearate(s) 0.03 Linoleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-VLDL-SM-pool(c) | 20 | - | - | - | - | - | - | - | 6 | - | - | - |
| 579 1-Acylglycerol-3P-VLDL-TG1-pool | 1-Acylglycerol-3P-VLDL-TG1-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-VLDL-TG1-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.003 Arachidonate(s) 0.7 Palmitate(s) 0.13 Oleate(s) 0.09 Stearate(s) 0.08 Linoleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-VLDL-TG1-pool(c) | 20 | - | - | - | - | - | - | - | 6 | - | - | - |
| 580 1-Acylglycerol-3P-arach | 1-Acylglycerol-3P-arach(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-arach | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Arachidonate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-arach(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 581 1-Acylglycerol-3P-lin | 1-Acylglycerol-3P-lin(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-lin | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Linoleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-lin(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 582 1-Acylglycerol-3P-ol | 1-Acylglycerol-3P-ol(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-ol | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Oleate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-ol(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 583 1-Acylglycerol-3P-palm | 1-Acylglycerol-3P-palm(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-palm | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Palmitate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-palm(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 584 1-Acylglycerol-3P-palmn | 1-Acylglycerol-3P-palmn(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-palmn | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Palmitolate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-palmn(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 585 1-Acylglycerol-3P-stea | 1-Acylglycerol-3P-stea(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-3P-stea | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Stearate(s) 2.5 ATP-energy(c) 1 NADH-redox-potential(c) | 1.5 $H_2O$(s) 1 1-Acylglycerol-3P-stea(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 586 1-Acylglycerol-VLDL-PC-pool | 1-Acylglycerol-VLDL-PC-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-VLDL-PC-pool | 0.5 Glucose-6P(c) 0.08 Arachidonate(s) 0.35 Palmitate(s) 0.14 Oleate(s) 0.15 Stearate(s) 0.27 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 1-Acylglycerol-VLDL-PC-pool(c) | 25 | - | - | - | - | - | - | - | 6 | - | - | - |
| 587 1-Acylglycerol-VLDL-PE-pool | 1-Acylglycerol-VLDL-PE-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-VLDL-PE-pool | 0.5 Glucose-6P(c) 0.3 Arachidonate(s) 0.17 Palmitate(s) 0.08 Oleate(s) 0.27 Stearate(s) 0.18 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 1-Acylglycerol-VLDL-PE-pool(c) | 25 | - | - | - | - | - | - | - | 6 | - | - | - |
| 588 1-Acylglycerol-VLDL-PI-pool | 1-Acylglycerol-VLDL-PI-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-VLDL-PI-pool | 0.5 Glucose-6P(c) 0.25 Arachidonate(s) 0.08 Palmitate(s) 0.16 Oleate(s) 0.43 Stearate(s) 0.08 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 1-Acylglycerol-VLDL-PI-pool(c) | 25 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 589 1-Acylglycerol-VLDL-PS-pool | 1-Acylglycerol-VLDL-PS-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-VLDL-PS-pool | 0.5 Glucose-6P(c) 0.27 Arachidonate(s) 0.04 Palmitate(s) 0.04 Oleate(s) 0.62 Stearate(s) 0.02 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 1-Acylglycerol-VLDL-PS-pool(c) | 25 | - | - | - | - | - | - | - | 6 | - | - | - |
| 590 1-Acylglycerol-VLDL-SM-pool | 1-Acylglycerol-VLDL-SM-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-VLDL-SM-pool | 0.5 Glucose-6P(c) 0.02 Arachidonate(s) 0.71 Palmitate(s) 0.07 Oleate(s) 0.17 Stearate(s) 0.03 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 1-Acylglycerol-VLDL-SM-pool(c) | 25 | - | - | - | - | - | - | - | 6 | - | - | - |
| 591 1-Acylglycerol-VLDL-TG1-pool | 1-Acylglycerol-VLDL-TG1-pool(c) | PIPES MCES | synthesis of cytosolic 1-Acylglycerol-VLDL-TG1-pool | 0.5 Glucose-6P(c) 0.003 Arachidonate(s) 0.7 Palmitate(s) 0.13 Oleate(s) 0.09 Stearate(s) 0.08 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $H_2O$(s) 0.5 $P_i$(c) 1 1-Acylglycerol-VLDL-TG1-pool(c) | 25 | - | - | - | - | - | - | - | 6 | - | - | - |
| 592 1-Pyrroline-5-carboxylate | 1-Pyrroline-5-carboxylate(c) | PIPES MCES | synthesis of cytosolic 1-Pyrroline-5-carboxylate | 1 Proline(s) | 1 1-Pyrroline-5-carboxylate(c) 1 NADPH-redox-potential(c) 1 Na-gradient(c) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |
| 593 14-Demethyllanosterol | 14-Demethyllanosterol(r) | PIPES MCES | synthesis of Golgi/ER 14-Demethyllanosterol | 4 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 6 NADPH-redox-potential(r) | 3 $H_2O$(s) 4 $P_i$(c) 1 $CO_2$(s) 1 14-Demethyllanosterol(r) 1 NADPH-redox-potential(c) | 5 | - | 7 | - | - | - | - | - | 3 | - | 4 | - |
| 594 2,5-Diamino-6-(5-triphosphoryl-3,4-trihydroxy-2-oxopentyl)- amino-4-oxopyrimidine | 2,5-Diamino-6-(5-triphosphoryl-3,4-trihydroxy-2-oxopentyl)-amino-4-oxopyrimidine(c) | PIPES MCES | synthesis of cytosolic 2,5-Diamino-6-(5-triphosphoryl-3,4-trihydroxy-2-oxopentyl)-amino-4-oxopyrimidine | 2.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 11.2 ATP-energy(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 2,5-Diamino-6-(5-triphosphoryl-3,4-trihydroxy-2-oxopentyl)- amino-4-oxopyrimidine(c) 2 NADH-redox-potential(c) 2 NADPH-redox-potential(c) | 40 | - | - | - | - | - | - | - | 6 | - | - | - |
| 595 2,5-Diaminopyrimidine(n)leoside triphosphate | 2,5-Diaminopyrimidine nleoside triphosphate(c) | PIPES MCES | synthesis of cytosolic 2,5-Diaminopyrimidine nleoside triphosphate | 2.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 11.2 ATP-energy(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 2,5-Diaminopyrimidine nleoside triphosphate(c) 2 NADH-redox-potential(c) 2 NADPH-redox-potential(c) | 39 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 596 2-Amino-3-carboxymuconate(s)semialdehyde | 2-Amino-3-carboxymuconate semialdehyde(c) | PIPES MCES | synthesis of cytosolic 2-Amino-3-carboxymuconate semialdehyde | 3 $O_2$(s) 1 Tryptophan(s) 1 ATP-energy(c) 1.5 NADPH-redox-potential(c) | 0.5 $CO_2$(s) 1 Alanine(s) 1 2-Amino-3-carboxymuconate semialdehyde(c) 1 Na-gradient(c) 0.5 THF-activated methyl group(c) | 13 | - | - | - | - | - | - | - | 5 | - | - | - |
| 597 2-Amino-3-oxoadipate | 2-Amino-3-oxoadipate(m) | PIPES MCES | synthesis of mitochondrial 2-Amino-3-oxoadipate | 0.5 Pyruvate(m) 1 Glutamate(s) 0.5 Serine(s) 0.5 NADPH-redox-potential(m) 0.5 Proton-gradient(m) | 0.5 Aspartate(s) 1 2-Amino-3-oxoadipate(m) 0.5 NADH-redox-potential(c) 1 NADH-redox-potential(m) 0.5 Proton-gradient(c) 1.5 Na-gradient(c) | 3 | 10 | - | - | - | - | - | - | 5 | - | 4 | - |
| 598 2-Aminomuconate | 2-Aminomuconate(c) | PIPES MCES | synthesis of cytosolic 2-Aminomuconate | 3 $O_2$(s) 1 Tryptophan(s) 1 ATP-energy(c) 3 NADPH-redox-potential(c) | 1 $CO_2$(s) 1 Alanine(s) 1 2-Aminomuconate(c) 1 NADH-redox-potential(c) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 15 | - | - | - | - | - | - | - | 5 | - | - | - |
| 599 2-Aminomuconate(s)semialdehyde | 2-Aminomuconate semialdehyde(c) | PIPES MCES | synthesis of cytosolic 2-Aminomuconate semialdehyde | 3 $O_2$(s) 1 Tryptophan(s) 1 ATP-energy(c) 1.5 NADPH-redox-potential(c) | 1.5 $CO_2$(s) 1 Alanine(s) 1 2-Aminomuconate semialdehyde(c) 1 Na-gradient(c) 0.5 THF-activated methyl group(c) | 14 | - | - | - | - | - | - | - | 5 | - | - | - |
| 600 2-Deoxy-D-ribose-1P | 2-Deoxy-D-ribose-1P(c) | PIPES MCES | synthesis of cytosolic 2-Deoxy-D-ribose-1P | 0.5 $P_i$(c) 1 Glutamate(s) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 2.5 ATP-energy(c) | 1.5 $H_2O$(s) 1 Glutamine(s) 1 2-Deoxy-D-ribose-1P(c) 1 Na-gradient(c) | 10 | - | - | - | - | - | - | - | 4 | - | - | - |
| 601 2-Deoxy-D-ribose-5P | 2-Deoxy-D-ribose-5P(c) | PIPES MCES | synthesis of cytosolic 2-Deoxy-D-ribose-5P | 0.5 $P_i$(c) 1 Glutamate(s) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 2.5 ATP-energy(c) | 1.5 $H_2O$(s) 1 Glutamine(s) 1 2-Deoxy-D-ribose-5P(c) 1 Na-gradient(c) | 9 | - | - | - | - | - | - | - | 4 | - | - | - |
| 602 2-Lysolecithin-pool | 2-Lysolecithin-pool(c) | PIPES MCES | synthesis of cytosolic 2-Lysolecithin-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Choline(c) 0.08 Arachidonate(s) 0.35 Palmitate(s) 0.14 Oleate(s) 0.15 Stearate(s) 0.27 Linoleate(s) 7.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 2-Lysolecithin-pool(c) | 30 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 603 2-Methylacetoacetyl-CoA | 2-Methylacetoacetyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 2-Methylacetoacetyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Threonine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 6.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 2-Methylacetoacetyl-CoA(m) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 5 Na-gradient(c) | 44 | 4 | - | - | - | - | - | - | 10 | - | 4 | - |
| 604 2-Methylbutyryl-CoA | 2-Methylbutyryl-CoA(m) | PIPES MCES | synthesis of mitochondrial 2-Methylbutyryl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Isoleucine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 2-Methylbutyryl-CoA(m) 1 NADH-redox-potential(m) 5.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 5 Na-gradient(c) | 42 | 5 | - | - | - | - | - | - | 10 | - | 6 | - |
| 605 2-Oxo-3-methylvalerate | 2-Oxo-3-methylvalerate(m) | PIPES MCES | synthesis of mitochondrial 2-Oxo-3-methylvalerate | 1 Glutamate(s) 1 Isoleucine(s) 1 ATP-energy(c) 1 Proton-gradient(m) | 1 Glutamine(s) 1 2-Oxo-3-methylvalerate(m) 1 NADH-redox-potential(m) 2 Na-gradient(c) | 2 | 3 | - | - | - | - | - | - | 4 | - | 4 | - |
| 606 2-Oxoadipate | 2-Oxoadipate(c) | PIPES MCES | synthesis of cytosolic 2-Oxoadipate | 1 Pyruvate(c) 1 Pyruvate(m) 0.5 Lysine(s) 0.5 NADH-redox-potential(m) | 1 Alanine(s) 1 2-Oxoadipate(c) 0.5 NADH-redox-potential(c) 1 Proton-gradient(m) | 3 | 10 | - | - | - | - | - | - | 2 | - | 8 | - |
| 607 2-Oxobutyrate | 2-Oxobutyrate(c) | PIPES MCES | synthesis of cytosolic 2-Oxobutyrate | 1 Glutamate(s) 1 Threonine(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Glutamine(s) 1 2-Oxobutyrate(c) 2 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 5 | - | - | - |
| 608 2-Oxoglutaramate | 2-Oxoglutaramate(c) | PIPES MCES | synthesis of cytosolic 2-Oxoglutaramate | 1 Pyruvate(c) 1 Glutamine(s) | 1 Alanine(s) 1 2-Oxoglutaramate(c) | 1 | - | - | - | - | - | - | - | 1 | - | - | - |
| 609 2PG | 2PG(c) | PIPES MCES | synthesis of cytosolic 2PG | 1 $P_i$(c) 1 Pyruvate(c) 1 ATP-energy(c) 1 NADPH-redox-potential(c) | 1 2PG(c) 1 NADH-redox-potential(c) | 8 | - | - | - | - | - | - | - | - | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 610 | 3(S)-3-hydroxydodecen-(5Z)-oyl-CoA | 3(S)-3-hydroxydodecen-(5Z)-oyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3(S)-3-hydroxydodecen-(5Z)-oyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 1 3(S)-3-hydroxydodecen-(5Z)-oyl-CoA(m) 3 Na-gradient(c) 2 CoA-activated acetyl group(m) | 44 | 12 | - | - | - | - | - | - | 11 | - | 3 | - |
| 611 | 3-Dehydrosphinganine | 3-Dehydrosphinganine(c) | PIPES MCES | synthesis of cytosolic 3-Dehydrosphinganine | 1 Serine(s) 1 Palmitate(s) 2 ATP-energy(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 3-Dehydrosphinganine(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 5 | - | - | - | - | - | - | - | 6 | - | - | - |
| 612 | 3-Hydroxy-L-kynurenine | 3-Hydroxy-L-kynurenine(c) | PIPES MCES | synthesis of cytosolic 3-Hydroxy-L-kynurenine | 2 $O_2$(s) 1 Tryptophan(s) 1 ATP-energy(c) | 1 $CO_2$(s) 1 3-Hydroxy-L-kynurenine(c) 1 Na-gradient(c) | 6 | - | - | - | - | - | - | - | 4 | - | - | - |
| 613 | 3-Hydroxyanthranilate | 3-Hydroxyanthranilate(c) | PIPES MCES | synthesis of cytosolic 3-Hydroxyanthranilate | 2 $O_2$(s) 1 Tryptophan(s) 1 ATP-energy(c) 1.5 NADPH-redox-potential(c) | 0.5 $CO_2$(s) 1 Alanine(s) 1 3-Hydroxyanthranilate(c) 1 Na-gradient(c) 0.5 THF-activated methyl group(c) | 12 | - | - | - | - | - | - | - | 5 | - | - | - |
| 614 | 3-Hydroxyisobutyrate | 3-Hydroxyisobutyrate(m) | PIPES MCES | synthesis of mitochondrial 3-Hydroxyisobutyrate | 0.67 $H_2O$(s) 0.5 $O_2$(s) 0.33 Glutamate(s) 1 Valine(s) 0.67 ATP-energy(c) 0.67 ATP-energy(m) | 0.67 $CO_2$(s) 0.33 Arginine(s) 1 3-Hydroxyisobutyrate(m) 0.33 NADH-redox-potential(c) 1 NADH-redox-potential(m) 4.33 Proton-gradient(m) 1.33 Na-gradient(c) | 9 | 12 | - | - | - | - | - | - | 7 | - | 10 | - |
| 615 | 3-Hydroxyisobutyryl-CoA | 3-Hydroxyisobutyryl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Hydroxyisobutyryl-CoA | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Valine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 3-Hydroxyisobutyryl-CoA(m) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 5 Proton-gradient(m) 4 Na-gradient(c) | 43 | 6 | - | - | - | - | - | - | 12 | - | 9 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 616 3-Hydroxypropionyl-CoA | 3-Hydroxypropionyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Hydroxypropionyl-CoA | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Threonine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 3-Hydroxypropionyl-CoA(m) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 5 Proton-gradient(m) 4 Na-gradient(c) | 44 | 4 | - | - | - | - | - | - | 12 | - | 7 | - |
| 617 3-Hydroxystearoyl-ACP | 3-Hydroxystearoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Hydroxystearoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 632 ATP-energy(c) 15 NADPH-redox-potential(c) 3 Proton-gradient(c) 9 CoA-activated acetyl group(c) | 10 $H_2O$(s) 1 $CO_2$(s) 1 3-Hydroxystearoyl-ACP(c) 66 Na-gradient(c) | 49 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 618 3-Keto-4-methylzymosterol | 3-Keto-4-methylzymosterol(r) | PIPES MCES | synthesis of Golgi/ER 3-Keto-4-methylzymosterol | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 9 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 2 $CO_2$(s) 1 3-Keto-4-methylzymosterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 10 | - | - | - | - | - | 3 | - | 5 | - |
| 619 3-Methyl-2-oxobutyrate | 3-Methyl-2-oxobutyrate(m) | PIPES MCES | synthesis of mitochondrial 3-Methyl-2-oxobutyrate | 1 Pyruvate(c) 1 Valine(s) 3 Proton-gradient(m) | 1 Alanine(s) 1 3-Methyl-2-oxobutyrate(m) 2 Na-gradient(c) | 1 | 1 | - | - | - | - | - | - | 3 | - | 6 | - |
| 620 3-Methylcrotonyl-CoA | 3-Methylcrotonyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Methylcrotonyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 2 THF-activated methyl group(c) 3 CoA-activated acetyl group(m) | 5.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3-Methylcrotonyl-CoA(m) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 Proton-gradient(c) 5 Na-gradient(c) | 42 | 7 | - | - | - | - | - | - | 10 | - | 2 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 621 3-Methylglutaconyl-CoA | 3-Methylglutaconyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Methylglutaconyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 2 THF-activated methyl group(c) 3 CoA-activated acetyl group(m) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3-Methylglutaconyl-CoA(m) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 Proton-gradient(c) 5 Na-gradient(c) | 42 | 4 | - | - | - | - | - | - | 10 | - | 1 | - |
| 622 3-Oxodecanoyl-ACP | 3-Oxodecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Oxodecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 628 ATP-energy(c) 6 NADPH-redox-potential(c) 3 Proton-gradient(c) 5 CoA-activated acetyl group(c) | 6 $H_2O$(s) 1 $CO_2$(s) 1 3-Oxodecanoyl-ACP(c) 66 Na-gradient(c) | 32 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 623 3-Oxodecanoyl-CoA | 3-Oxodecanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Oxodecanoyl-CoA | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3-Oxodecanoyl-CoA(m) 2 NADH-redox-potential(c) 5 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 6 Proton-gradient(m) 3 Na-gradient(c) 4 CoA-activated acetyl group(m) | 44 | 21 | - | - | - | - | - | - | 12 | - | 7 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | | Definition | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 624 | 3-Oxododecanoyl-ACP | 3-Oxododecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Oxododecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 629 ATP-energy(c) 8 NADPH-redox-potential(c) 3 Proton-gradient(c) 6 CoA-activated acetyl group(c) | 7 $H_2O$(s) 1 $CO_2$(s) 1 3-Oxododecanoyl-ACP(c) 66 Na-gradient(c) | 36 | - | - | - | - | - | - | - | 24 | - | - | 1 | |
| 625 | 3-Oxododecanoyl-CoA | 3-Oxododecanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Oxododecanoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3-Oxododecanoyl-CoA(m) 2 NADH-redox-potential(c) 4 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 3 Na-gradient(c) 3 CoA-activated acetyl group(m) | 44 | 17 | - | - | - | - | - | - | 11 | - | 3 | - | |
| 626 | 3-Oxohexadecanoyl-ACP | 3-Oxohexadecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Oxohexadecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 631 ATP-energy(c) 12 NADPH-redox-potential(c) 3 Proton-gradient(c) 8 CoA-activated acetyl group(c) | 9 $H_2O$(s) 1 $CO_2$(s) 1 3-Oxohexadecanoyl-ACP(c) 66 Na-gradient(c) | 44 | - | - | - | - | - | - | - | 24 | - | - | 1 | |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 627 3-Oxohexanoyl-ACP | 3-Oxohexanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Oxohexanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 626 ATP-energy(c) 2 NADPH-redox-potential(c) 3 CoA-activated acetyl group(c) | 4 $H_2O$(s) 1 $CO_2$(s) 1 3-Oxohexanoyl-ACP(c) 2 Proton-gradient(c) 82 Na-gradient(c) | 24 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 628 3-Oxohexanoyl-CoA | 3-Oxohexanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Oxohexanoyl-CoA | 1.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3-Oxohexanoyl-CoA(m) 2 NADH-redox-potential(c) 7 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 1 Proton-gradient(c) 18 Proton-gradient(m) 5 Na-gradient(c) 6 CoA-activated acetyl group(m) | 44 | 29 | - | - | - | - | - | - | 12 | - | 7 | - |
| 629 3-Oxooctanoyl-ACP | 3-Oxooctanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Oxooctanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 627 ATP-energy(c) 4 NADPH-redox-potential(c) 3 Proton-gradient(c) 4 CoA-activated acetyl group(c) | 5 $H_2O$(s) 1 $CO_2$(s) 1 3-Oxooctanoyl-ACP(c) 66 Na-gradient(c) | 28 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 630 3-Oxooctanoyl-CoA | 3-Oxooctanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Oxooctanoyl-CoA | 1 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3-Oxooctanoyl-CoA(m) 2 NADH-redox-potential(c) 6 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 12 Proton-gradient(m) 3 Na-gradient(c) 5 CoA-activated acetyl group(m) | 44 | 25 | - | - | - | - | - | - | 11 | - | 7 | - |
| 631 3-Oxopalmitoyl-CoA | 3-Oxopalmitoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Oxopalmitoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 0.5 Aspartate(s) 0.5 Glutamine(s) 0.83 Glucose-6P(c) 1.5 Asparagine(s) 0.5 Palmitate(s) 0.5 Cystine(s) 1 Pantothenate(s) 0.5 Palmitolate(s) 14.7 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 3-Oxopalmitoyl-CoA(m) 2.5 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 6 Proton-gradient(m) 1.5 Na-gradient(c) | 49 | 5 | - | - | - | - | - | - | 12 | - | 6 | - |
| 632 3-Oxopropanoate | 3-Oxopropanoate(m) | PIPES MCES | synthesis of mitochondrial 3-Oxopropanoate | 1 Pyruvate(c) 1 NADPH-redox-potential(c) 2 Proton-gradient(m) | 1 3-Oxopropanoate(m) 1 NADH-redox-potential(c) | 6 | 1 | - | - | - | - | - | - | - | - | 6 | - |
| 633 3-Oxostearoyl-ACP | 3-Oxostearoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Oxostearoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 632 ATP-energy(c) 14 NADPH-redox-potential(c) 3 Proton-gradient(c) 9 CoA-activated acetyl group(c) | 10 $H_2O$(s) 1 $CO_2$(s) 1 3-Oxostearoyl-ACP(c) 66 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | | Definition | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 634 | 3-Oxotetradecanoyl-ACP | 3-Oxotetradecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic 3-Oxotetradecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 630 ATP-energy(c) 10 NADPH-redox-potential(c) 3 Proton-gradient(c) 7 CoA-activated acetyl group(c) | 8 $H_2O$(s) 1 $CO_2$(s) 1 3-Oxotetradecanoyl-ACP(c) 66 Na-gradient(c) | 40 | - | - | - | - | - | - | - | 24 | - | - | 1 | |
| 635 | 3-Oxotetradecanoyl-CoA | 3-Oxotetradecanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-Oxotetradecanoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 0.5 Aspartate(s) 0.5 Glutamine(s) 0.83 Glucose-6P(c) 1.5 Asparagine(s) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 14.7 ATP-energy(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 3-Oxotetradecanoyl-CoA(m) 3 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 12 Proton-gradient(m) 1.5 Na-gradient(c) 1 CoA-activated acetyl group(m) | 48 | 10 | - | - | - | - | - | - | 10 | - | 6 | - | |
| 636 | 3-Phosphonooxypyruvate | 3-Phosphonooxypyruvate(c) | PIPES MCES | synthesis of cytosolic 3-Phosphonooxypyruvate | 0.67 $P_i$(c) 0.33 Pyruvate(c) 0.33 Serine(s) 0.33 Glucose-6P(c) 0.33 NADPH-redox-potential(c) | 0.33 Alanine(s) 1 3-Phosphonooxypyruvate(c) 1.67 NADH-redox-potential(c) 0.33 Proton-gradient(c) 0.33 Na-gradient(c) | 12 | - | - | - | - | - | - | - | 4 | - | - | - | |
| 637 | 3-Phosphoserine | 3-Phosphoserine(c) | PIPES MCES | synthesis of cytosolic 3-Phosphoserine | 0.67 $P_i$(c) 0.67 Alanine(s) 0.33 Serine(s) 0.33 Glucose-6P(c) 0.33 NADPH-redox-potential(c) 0.33 Proton-gradient(c) | 0.67 Pyruvate(c) 1 3-Phosphoserine(c) 1.67 NADH-redox-potential(c) 0.33 Na-gradient(c) | 14 | - | - | - | - | - | - | - | 4 | - | - | - | |
| 638 | 3-Sulfinoalanine | 3-Sulfinoalanine(c) | PIPES MCES | synthesis of cytosolic 3-Sulfinoalanine | 1 $O_2$(s) 1 Cysteine(s) | 1 3-Sulfinoalanine(c) | 1 | - | - | - | - | - | - | - | 2 | - | - | - | |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | | Definition | | Solution | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | |
| 639 | 3-Ureidoisobutyrate | 3-Ureidoisobutyrate(c) | PIPES MCES | synthesis of cytosolic 3-Ureidoisobutyrate | 0.33 $O_2$(s) 1 Aspartate(s) 1 Glutamine(s) 0.33 Proline(s) 4 ATP-energy(c) 2 NADH-redox-potential(c) 1 THF-activated methyl group(c) | 1.33 Glutamate(s) 1 3-Ureidoisobutyrate(c) 0.33 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Proton-gradient(c) 4 Proton-gradient(m) 2.33 Na-gradient(c) | 26 | 4 | - | - | - | - | - | - | 7 | - | 6 | - | |
| 640 | 3-Ureidopropionate | 3-Ureidopropionate(c) | PIPES MCES | synthesis of cytosolic 3-Ureidopropionate | 0.33 $O_2$(s) 1 Aspartate(s) 1 Glutamine(s) 0.33 Proline(s) 3 ATP-energy(c) 1 NADPH-redox-potential(c) | 1.33 Glutamate(s) 1 3-Ureidopropionate(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 17 | 4 | - | - | - | - | - | - | 6 | - | 6 | - | |
| 641 | 3-oxolaur-cis-5-enoyl-CoA | 3-oxolaur-cis-5-enoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-oxolaur-cis-5-enoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 1 3-oxolaur-cis-5-enoyl-CoA(m) 3 Na-gradient(c) 2 CoA-activated acetyl group(m) | 44 | 13 | - | - | - | - | - | - | 11 | - | 3 | - | |
| 642 | 3-oxomyrist-7-enoyl-CoA | 3-oxomyrist-7-enoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-oxomyrist-7-enoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 FADH-redox-potential(c) 1 3-oxomyrist-7-enoyl-CoA(m) 3 Na-gradient(c) 1 CoA-activated acetyl group(m) | 44 | 9 | - | - | - | - | - | - | 11 | - | 3 | - | |
| 643 | 3-oxooleoyl-CoA | 3-oxooleoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-oxooleoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(m) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 3-oxooleoyl-CoA(m) 3 Na-gradient(c) | 43 | 2 | - | - | - | - | - | - | 11 | - | 1 | - | |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | | Definition | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 644 | 3-oxopalmitoleoyl-CoA | 3-oxopalmitoleoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial 3-oxopalmitoleoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 1 FADH-redox-potential(c) 1 3-oxopalmitoleoyl-CoA(m) 3 Na-gradient(c) | 44 | 4 | - | - | - | - | - | - | 11 | - | 3 | - |
| 645 | 3PG | 3PG(c) | PIPES MCES | synthesis of cytosolic 3PG | 0.67 $P_i$(c) 0.33 Pyruvate(c) 0.33 Serine(s) 0.33 Glucose-6P(c) 0.33 NADPH-redox-potential(c) | 0.33 Alanine(s) 1 3PG(c) 0.67 NADH-redox-potential(c) 0.33 Proton-gradient(c) 0.33 Na-gradient(c) | 11 | - | - | - | - | - | - | - | 4 | - | - | - |
| 646 | 3alpha,7alpha,12alpha,24-Tetrahydroxy-5beta-cholestanoyl-CoA | 3alpha,7alpha,12alpha,24-Tetrahydroxy-5beta-cholestanoyl-CoA(p) | PIPES MCES | synthesis of peroxysomal 3alpha,7alpha,12alpha,24-Tetrahydroxy-5beta-cholestanoyl-CoA | 11.5 $O_2$(s) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 2 Farnesyl-PP(r) 0.5 Cystine(s) 1 Pantothenate(s) 15.2 ATP-energy(c) 12 NADPH-redox-potential(r) 0.5 NADPH-redox-potential(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 17.2 $H_2O$(s) 1.83 $P_i$(c) 4 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3alpha,7alpha,12alpha,24-Tetrahydroxy-5beta-cholestanoyl-CoA(p) 1 NADH-redox-potential(r) 3 NADH-redox-potential(c) 5 Na-gradient(c) | 48 | - | 19 | 4 | - | - | - | - | 11 | - | 11 | - |
| 647 | 3alpha,7alpha,12alpha-Trihydroxy-5beta-24-oxocholestanoyl-CoA | 3alpha,7alpha,12alpha-Trihydroxy-5beta-24-oxocholestanoyl-CoA(p) | PIPES MCES | synthesis of peroxysomal 3alpha,7alpha,12alpha-Trihydroxy-5beta-24-oxocholestanoyl-CoA | 11.5 $O_2$(s) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 2 Farnesyl-PP(r) 0.5 Cystine(s) 1 Pantothenate(s) 15.2 ATP-energy(c) 12 NADPH-redox-potential(r) 0.5 NADPH-redox-potential(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 17.2 $H_2O$(s) 1.83 $P_i$(c) 4 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3alpha,7alpha,12alpha-Trihydroxy-5beta-24-oxocholestanoyl-CoA(p) 1 NADH-redox-potential(r) 3 NADH-redox-potential(c) 1 NADH-redox-potential(p) 5 Na-gradient(c) | 48 | - | 19 | 6 | - | - | - | - | 11 | - | 11 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 648 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholest-24-enoyl-CoA | 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholest-24-enoyl-CoA(p) | PIPES MCES | synthesis of peroxysomal 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholest-24-enoyl-CoA | 11.5 $O_2$(s) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Calbose-6P(c) 2 Farnesyl-PP(r) 0.5 Cystine(s) 1 Pantothenate(s) 15.2 ATP-energy(c) 12 NADPH-redox-potential(r) 0.5 NADPH-redox-potential(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 18.2 $H_2O$(s) 1.83 $P_i$(c) 4 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholest-24-enoyl-CoA(p) 1 NADH-redox-potential(r) 3 NADH-redox-potential(c) 3 Na-gradient(c) | 48 | - | 19 | 4 | - | - | - | - | 11 | - | 11 | - |
| 649 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-al | 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-al(c) | PIPES MCES | synthesis of cytosolic 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-al | 11 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 12 NADPH-redox-potential(r) 2 NADPH-redox-potential(c) | 10 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-al(c) 1 NADH-redox-potential(r) 1 NADH-redox-potential(c) | 10 | - | 19 | - | - | - | - | - | 3 | - | 6 | - |
| 650 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanate | 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanate(c) | PIPES MCES | synthesis of cytosolic 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanate | 11 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 12 NADPH-redox-potential(r) 2 NADPH-redox-potential(c) | 9 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanate(c) 1 NADH-redox-potential(r) 2 NADH-redox-potential(c) | 11 | - | 19 | - | - | - | - | - | 3 | - | 6 | - |
| 651 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA | 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA(r) | PIPES MCES | synthesis of Golgi/ER 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA | 11 $O_2$(s) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Calbose-6P(c) 2 Farnesyl-PP(r) 0.5 Cystine(s) 1 Pantothenate(s) 14.2 ATP-energy(c) 12 NADPH-redox-potential(r) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 17.2 $H_2O$(s) 1.83 $P_i$(c) 4 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA(r) 1 NADH-redox-potential(r) 2 NADH-redox-potential(c) 0.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | 20 | - | - | - | - | - | 11 | - | 9 | - |
| 652 3alpha,7alpha,12alpha-Trihydroxycoprostane | 3alpha,7alpha,12alpha-Trihydroxycoprostane(c) | PIPES MCES | synthesis of cytosolic 3alpha,7alpha,12alpha-Trihydroxycoprostane | 10 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 12 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) | 9 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 3alpha,7alpha,12alpha-Trihydroxycoprostane(c) 1 NADH-redox-potential(r) | 7 | - | 19 | - | - | - | - | - | 3 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 653 3alpha,7alpha-Dihydroxy-5beta-cholestan-26-al | 3alpha,7alpha-Dihydroxy-5beta-cholestan-26-al(c) | PIPES MCES | synthesis of cytosolic 3alpha,7alpha-Dihydroxy-5beta-cholestan-26-al | 10 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 9 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 3alpha,7alpha-Dihydroxy-5beta-cholestan-26-al(c) 1 NADH-redox-potential(r) 1 NADH-redox-potential(c) | 9 | 2 | 18 | - | - | - | - | - | 3 | - | 10 | - |
| 654 3alpha,7alpha-Dihydroxy-5beta-cholestanate | 3alpha,7alpha-Dihydroxy-5beta-cholestanate(c) | PIPES MCES | synthesis of cytosolic 3alpha,7alpha-Dihydroxy-5beta-cholestanate | 10 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 3alpha,7alpha-Dihydroxy-5beta-cholestanate(c) 1 NADH-redox-potential(r) 2 NADH-redox-potential(c) | 10 | 2 | 18 | - | - | - | - | - | 3 | - | 10 | - |
| 655 3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA | 3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA(r) | PIPES MCES | synthesis of Golgi/ER 3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA | 10 $O_2$(s) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 2 Farnesyl-PP(r) 0.5 Cystine(s) 1 Pantothenate(s) 14.2 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(m) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 16.2 $H_2O$(s) 1.83 $P_i$(c) 4 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA(r) 1 NADH-redox-potential(r) 3 NADH-redox-potential(c) 0.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 47 | 2 | 19 | - | - | - | - | - | 11 | - | 13 | - |
| 656 4,4-Dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol | 4,4-Dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol(r) | PIPES MCES | synthesis of Golgi/ER 4,4-Dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol | 4 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 5 NADPH-redox-potential(r) | 3 $H_2O$(s) 4 $P_i$(c) 1 $CO_2$(s) 1 4,4-Dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol(r) 1 NADPH-redox-potential(c) | 5 | - | 6 | - | - | - | - | - | 3 | - | 4 | - |
| 657 4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate | 4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate(c) | PIPES MCES | synthesis of cytosolic 4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate | 2 $O_2$(s) 1 Pyruvate(c) 1 Tryptophan(s) 1 ATP-energy(c) | 1 $CO_2$(s) 1 Alanine(s) 1 4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate(c) 1 Na-gradient(c) | 8 | - | - | - | - | - | - | - | 5 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 658 4-Hydroxyphenylpyruvate | 4-Hydroxyphenylpyruvate(c) | PIPES MCES | synthesis of cytosolic 4-Hydroxyphenylpyruvate | 1 Pyruvate(c) 1 Tyrosine(s) | 1 Alanine(s) 1 4-Hydroxyphenylpyruvate(c) 1 Na-gradient(c) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 659 4-Imidazolone-5-propanoate | 4-Imidazolone-5-propanoate(c) | PIPES MCES | synthesis of cytosolic 4-Imidazolone-5-propanoate | 1 Glutamate(s) 1 Histidine(s) 1 ATP-energy(c) | 1 Glutamine(s) 1 4-Imidazolone-5-propanoate(c) 1 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 4 | - | - | - |
| 660 4-Maleylacetoacetate | 4-Maleylacetoacetate(c) | PIPES MCES | synthesis of cytosolic 4-Maleylacetoacetate | 2 $O_2$(s) 1 Pyruvate(c) 1 Tyrosine(s) | 1 $CO_2$(s) 1 Alanine(s) 1 4-Maleylacetoacetate(c) 1 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 5 | - | - | - |
| 661 4-Methyl-2-oxopentanoate | 4-Methyl-2-oxopentanoate(m) | PIPES MCES | synthesis of mitochondrial 4-Methyl-2-oxopentanoate | 0.4 Pyruvate(m) 0.6 Leucine(s) 0.2 ATP-energy(c) 0.6 NADH-redox-potential(m) 0.2 Proton-gradient(m) 1.6 CoA-activated acetyl group(m) | 0.2 Glutamine(s) 0.2 Proline(s) 1 4-Methyl-2-oxopentanoate(m) 0.4 NADPH-redox-potential(m) 0.6 Na-gradient(c) | 2 | 19 | - | - | - | - | - | - | 5 | - | 7 | - |
| 662 4alpha-Methylzymosterol | 4alpha-Methylzymosterol(r) | PIPES MCES | synthesis of Golgi/ER 4alpha-Methylzymosterol | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 8 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 2 $CO_2$(s) 1 4alpha-Methylzymosterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 11 | - | - | - | - | - | 3 | - | 5 | - |
| 663 4alpha-Methylzymosterol-4-carboxylate | 4alpha-Methylzymosterol-4-carboxylate(r) | PIPES MCES | synthesis of Golgi/ER 4alpha-Methylzymosterol-4-carboxylate | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 9 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 1 $CO_2$(s) 1 4alpha-Methylzymosterol-4-carboxylate(r) 1 NADPH-redox-potential(c) | 5 | - | 8 | - | - | - | - | - | 3 | - | 4 | - |
| 664 5,10-Methenyl-THF | 5,10-Methenyl-THF(c) | PIPES MCES | synthesis of cytosolic 5,10-Methenyl-THF | 1 Folate(s) 1 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 1 5,10-Methenyl-THF(c) 1 NADH-redox-potential(c) | 7 | - | - | - | - | - | - | - | 1 | - | - | - |
| 665 5,6-Dihydrouracil | 5,6-Dihydrouracil(c) | PIPES MCES | synthesis of cytosolic 5,6-Dihydrouracil | 0.33 $O_2$(s) 1 Aspartate(s) 1 Glutamine(s) 0.33 Proline(s) 3 ATP-energy(c) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1.33 Glutamate(s) 1 5,6-Dihydrouracil(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 16 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 666 5-Aminolevulinate | 5-Aminolevulinate(c) | PIPES MCES | synthesis of cytosolic 5-Aminolevulinate | 0.5 Pyruvate(m) 1 Glutamate(s) 0.5 Serine(s) 1 Proton-gradient(m) | 1 $CO_2$(s) 0.5 Aspartate(s) 1 5-Aminolevulinate(c) 1 NADH-redox-potential(m) 1 Na-gradient(c) | - | 9 | - | - | - | - | - | - | 5 | - | 6 | - |
| 667 5-Formiminotetrahydrofolate | 5-Formiminotetrahydrofolate(c) | PIPES MCES | synthesis of cytosolic 5-Formiminotetrahydrofolate | 1 $NH_3$(s) 1 Folate(s) 1 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 1 5-Formiminotetrahydrofolate(c) 1 NADH-redox-potential(c) | 8 | - | - | - | - | - | - | - | 2 | - | - | - |
| 668 5-Formyl-THF | 5-Formyl-THF(m) | PIPES MCES | synthesis of mitochondrial 5-Formyl-THF | 1 $H_2O$(s) 3.5 $O_2$(s) 1 Glutamate(s) 1 Tryptophan(s) 1 Folate(s) 1 ATP-energy(c) 1 ATP-energy(m) 2 NADPH-redox-potential(c) 2 NADPH-redox-potential(m) | 3 $CO_2$(s) 1 Alanine(s) 1 Glutamine(s) 1 5-Formyl-THF(m) 1 NADH-redox-potential(c) 2 NADH-redox-potential(m) 5 Proton-gradient(m) 2 Na-gradient(c) 2 CoA-activated acetyl group(m) | 12 | 14 | - | - | - | - | - | - | 9 | - | 11 | - |
| 669 5-Hydroxy-L-tryptophan | 5-Hydroxy-L-tryptophan(c) | PIPES MCES | synthesis of cytosolic 5-Hydroxy-L-tryptophan | 1 $O_2$(s) 1 Tryptophan(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 5-Hydroxy-L-tryptophan(c) 1 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 4 | - | - | - |
| 670 5-Methyl-THF | 5-Methyl-THF(c) | PIPES MCES | synthesis of cytosolic 5-Methyl-THF | 1 Folate(s) 2 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 1 5-Methyl-THF(c) | 4 | - | - | - | - | - | - | - | 1 | - | - | - |
| 671 5-Methylthioadenosine | 5-Methylthioadenosine(c) | PIPES MCES | synthesis of cytosolic 5-Methylthioadenosine | 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 1 Methionine(s) 0.83 Glucose-6P(c) 9.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 0.83 $P_i$(c) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 5-Methylthioadenosine(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Adenosylmethioninamine-potential(c) 3 Na-gradient(c) | 37 | - | - | - | - | - | - | - | 9 | - | - | - |
| 672 5-Oxoproline | 5-Oxoproline(c) | PIPES MCES | synthesis of cytosolic 5-Oxoproline | 1 Glutamate(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 5-Oxoproline(c) 1 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 3 | - | - | - |
| 673 5-Phosphoribosyl-4-carboxy-5-aminoimidazole | 5-Phosphoribosyl-4-carboxy-5-aminoimidazole(c) | PIPES MCES | synthesis of cytosolic 5-Phosphoribosyl-4-carboxy-5-aminoimidazole | 1 Glycine(s) 2 Glutamine(s) 1 Glucose-6P(c) 5 ATP-energy(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 2 Glutamate(s) 1 5-Phosphoribosyl-4-carboxy-5-aminoimidazole(c) 1 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 20 | - | - | - | - | - | - | - | 4 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | | Definition | | Solution | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | | | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn | | |
| 674 | 5-Phosphoribosylamine | 5-Phosphoribosylamine(c) | PIPES MCES | synthesis of cytosolic 5-Phosphoribosylamine | 0.17 $P_i$(c) 1 Glutamine(s) 0.83 Glucose-6P(c) 2.17 ATP-energy(c) | 0.17 $H_2O$(s) 1 Glutamate(s) 1 5-Phosphoribosylamine(c) | 14 | - | - | - | - | - | - | - | 3 | - | - | - | |
| 675 | 5-Phosphoribosylformylglycinamidine | 5-Phosphoribosylformylglycinamidine(c) | PIPES MCES | synthesis of cytosolic 5-Phosphoribosylformylglycinamidine | 0.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 4.17 ATP-energy(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 0.17 $H_2O$(s) 2 Glutamate(s) 1 5-Phosphoribosylformylglycinamidine(c) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) | 23 | - | - | - | - | - | - | - | 5 | - | - | - | |
| 676 | 5alpha-Cholesta-7,24-dien-3beta-ol | 5alpha-Cholesta-7,24-dien-3beta-ol(r) | PIPES MCES | synthesis of Golgi/ER 5alpha-Cholesta-7,24-dien-3beta-ol | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 8 NADPH-redox-potential(r) | 5 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 5alpha-Cholesta-7,24-dien-3beta-ol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 13 | - | - | - | - | - | 3 | - | 5 | - | |
| 677 | 5beta-Cholestane-3alpha,7alpha,12alpha,26-tetrol | 5beta-Cholestane-3alpha,7alpha,12alpha,26-tetrol(c) | PIPES MCES | synthesis of cytosolic 5beta-Cholestane-3alpha,7alpha,12alpha,26-tetrol | 11 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 12 NADPH-redox-potential(r) 2 NADPH-redox-potential(c) | 10 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 5beta-Cholestane-3alpha,7alpha,12alpha,26-tetrol(c) 1 NADH-redox-potential(r) | 8 | - | 19 | - | - | - | - | - | 3 | - | 6 | - | |
| 678 | 5beta-Cholestane-3alpha,7alpha,26-triol | 5beta-Cholestane-3alpha,7alpha,26-triol(c) | PIPES MCES | synthesis of cytosolic 5beta-Cholestane-3alpha,7alpha,26-triol | 10 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) | 9 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 5beta-Cholestane-3alpha,7alpha,26-triol(c) 1 NADH-redox-potential(r) | 6 | 2 | 19 | - | - | - | - | - | 3 | - | 10 | - | |
| 679 | 5beta-Cholestane-3alpha,7alpha-diol | 5beta-Cholestane-3alpha,7alpha-diol(c) | PIPES MCES | synthesis of cytosolic 5beta-Cholestane-3alpha,7alpha-diol | 9 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 5beta-Cholestane-3alpha,7alpha-diol(c) 1 NADH-redox-potential(r) | 7 | - | 18 | - | - | - | - | - | 3 | - | 6 | - | |
| 680 | 6-Phospho-D-gluconate | 6-Phospho-D-gluconate(c) | PIPES MCES | synthesis of cytosolic 6-Phospho-D-gluconate | 1 $H_2O$(s) 1 Glucose-6P(c) | 1 6-Phospho-D-gluconate(c) 1 NADPH-redox-potential(c) | 3 | - | - | - | - | - | - | - | 1 | - | - | - | |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 681 6-Pyruvoyltetrahydropterin | 6-Pyruvoyltetrahydropterin(c) | PIPES MCES | synthesis of cytosolic 6-Pyruvoyltetrahydropterin | 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 11.2 ATP-energy(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 1.17 $H_2O$(s) 0.83 $P_i$(c) 1 Pyruvate(c) 2 Glutamate(s) 1 6-Pyruvoyltetrahydropterin(c) 2 NADH-redox-potential(c) 2 NADPH-redox-potential(c) | 40 | - | - | - | - | - | - | - | 6 | - | - | - |
| 682 7-Dehydrodesmosterol | 7-Dehydrodesmosterol(r) | PIPES MCES | synthesis of Golgi/ER 7-Dehydrodesmosterol | 8 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 9 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 7-Dehydrodesmosterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 14 | - | - | - | - | - | 3 | - | 5 | - |
| 683 7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one | 7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one(c) | PIPES MCES | synthesis of cytosolic 7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one | 10 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 12 NADPH-redox-potential(r) | 9 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one(c) 1 NADH-redox-potential(r) | 5 | - | 19 | - | - | - | - | - | 3 | - | 6 | - |
| 684 7alpha,12alpha-Dihydroxycholest-4-en-3-one | 7alpha,12alpha-Dihydroxycholest-4-en-3-one(c) | PIPES MCES | synthesis of cytosolic 7alpha,12alpha-Dihydroxycholest-4-en-3-one | 10 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 12 NADPH-redox-potential(r) | 9 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 7alpha,12alpha-Dihydroxycholest-4-en-3-one(c) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 19 | - | - | - | - | - | 3 | - | 6 | - |
| 685 7alpha-Hydroxy-5beta-cholestan-3-one | 7alpha-Hydroxy-5beta-cholestan-3-one(c) | PIPES MCES | synthesis of cytosolic 7alpha-Hydroxy-5beta-cholestan-3-one | 9 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 11 NADPH-redox-potential(r) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 7alpha-Hydroxy-5beta-cholestan-3-one(c) 1 NADH-redox-potential(r) | 5 | - | 18 | - | - | - | - | - | 3 | - | 6 | - |
| 686 7alpha-Hydroxycholest-4-en-3-one | 7alpha-Hydroxycholest-4-en-3-one(c) | PIPES MCES | synthesis of cytosolic 7alpha-Hydroxycholest-4-en-3-one | 9 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 11 NADPH-redox-potential(r) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 7alpha-Hydroxycholest-4-en-3-one(c) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 18 | - | - | - | - | - | 3 | - | 6 | - |
| 687 7alpha-Hydroxycholesterol | 7alpha-Hydroxycholesterol(r) | PIPES MCES | synthesis of Golgi/ER 7alpha-Hydroxycholesterol | 9 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 12 NADPH-redox-potential(r) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 7alpha-Hydroxycholesterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 17 | - | - | - | - | - | 3 | - | 5 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 688 ACP | ACP(c) | PIPES MCES | synthesis of cytosolic ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 624 ATP-energy(c) 9 Proton-gradient(c) | 3 $H_2O$(s) 1 $CO_2$(s) 1 ACP(c) 82 Na-gradient(c) | 12 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 689 ADP | ADP(c) | PIPES MCES | synthesis of ADP | 1.17 $P_i$(c) 1 Glycine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 10.2 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 ADP(c) 1 $CO_2$(s) 2 Pyruvate(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 36 | - | - | - | - | - | - | - | 6 | - | - | - |
| 690 AICAR | AICAR(c) | PIPES MCES | synthesis of cytosolic AICAR | 0.17 $P_i$(c) 1 Glycine(s) 1 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 6.17 ATP-energy(c) 1 THF-activated methyl group(c) | 1.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 AICAR(c) 1 NADH-redox-potential(c) 2 NADPH-redox-potential(c) 2 Proton-gradient(c) 3 Na-gradient(c) | 29 | - | - | - | - | - | - | - | 7 | - | - | - |
| 691 AIR | AIR(c) | PIPES MCES | synthesis of cytosolic AIR | 0.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 5.17 ATP-energy(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 1.17 $H_2O$(s) 2 Glutamate(s) 1 AIR(c) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) | 24 | - | - | - | - | - | - | - | 5 | - | - | - |
| 692 AMP | AMP(c) | PIPES MCES | synthesis of AMP | 0.17 $P_i$(c) 1 Glycine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 9.17 ATP-energy(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 1 $CO_2$(s) 1 AMP(c) 2 Pyruvate(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 36 | - | - | - | - | - | - | - | 6 | - | - | - |
| 693 Acetaldehyde | Acetaldehyde(s) | PIPES MCES | synthesis of Acetaldehyde and blood export | 1 Glutamate(s) 1 Ethanolamine(c) 2 ATP-energy(c) | 1 $H_2O$(s) 1 Glutamine(s) 1 Acetaldehyde(s) 1 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 5 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 694 Acetate | Acetate(s) | PIPES MCES | synthesis of Acetate and blood export | 1 $H_2O$(s) 1 CoA-activated acetyl group(c) | 1 Acetate(s) 1 Proton-gradient(c) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 695 Acetoacetyl-ACP | Acetoacetyl-ACP(c) | PIPES MCES | synthesis of cytosolic Acetoacetyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 625 ATP-energy(c) 9 Proton-gradient(c) 2 CoA-activated acetyl group(c) | 3 $H_2O$(s) 1 $CO_2$(s) 1 Acetoacetyl-ACP(c) 82 Na-gradient(c) | 19 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 696 Acetoacetyl-CoA | Acetoacetyl-CoA(c) | PIPES MCES | synthesis of cytosolic Acetoacetyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 2 CoA-activated acetyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acetoacetyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 44 | - | - | - | - | - | - | - | 10 | - | - | - |
| 697 Acetyl-ACP | Acetyl-ACP(c) | PIPES MCES | synthesis of cytosolic Acetyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 624 ATP-energy(c) 9 Proton-gradient(c) 1 CoA-activated acetyl group(c) | 3 $H_2O$(s) 1 $CO_2$(s) 1 Acetyl-ACP(c) 82 Na-gradient(c) | 14 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 698 Acetyl-CoA | Acetyl-CoA(c) | PIPES MCES | synthesis of cytosolic Acetyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 1 Acetyl-CoA(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 10 | - | - | - |
| 699 Acrylyl-CoA | Acrylyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Acrylyl-CoA | 0.33 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Threonine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 1.33 Glutamate(s) 1 Acrylyl-CoA(m) 2 NADH-redox-potential(c) 1.33 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 Proton-gradient(m) 4.33 Na-gradient(c) | 44 | 6 | - | - | - | - | - | - | 13 | - | 8 | - |
| 700 Acyl-CoA-Bile-PC-pool | Acyl-CoA-Bile-PC-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-Bile-PC-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.06 Arachidonate(s) 0.41 Palmitate(s) 0.5 Cystine(s) 0.12 Oleate(s) 1 Pantothenate(s) 0.05 Stearate(s) 0.33 Linoleate(s) 0.03 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-Bile-PC-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 49 | - | - | - | - | - | - | - | 16 | - | - | - |
| 701 Acyl-CoA-CL-pool | Acyl-CoA-CL-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-CL-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.04 Palmitate(s) 0.5 Cystine(s) 0.14 Oleate(s) 1 Pantothenate(s) 0.02 Stearate(s) 0.75 Linoleate(s) 0.05 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-CL-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 702 Acyl-CoA-VLDL-PC-pool | Acyl-CoA-VLDL-PC-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-VLDL-PC-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.08 Arachidonate(s) 0.35 Palmitate(s) 0.5 Cystine(s) 0.14 Oleate(s) 1 Pantothenate(s) 0.15 Stearate(s) 0.27 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-VLDL-PC-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |
| 703 Acyl-CoA-VLDL-PE-pool | Acyl-CoA-VLDL-PE-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-VLDL-PE-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.3 Arachidonate(s) 0.17 Palmitate(s) 0.5 Cystine(s) 0.08 Oleate(s) 1 Pantothenate(s) 0.27 Stearate(s) 0.18 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-VLDL-PE-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |
| 704 Acyl-CoA-VLDL-PI-pool | Acyl-CoA-VLDL-PI-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-VLDL-PI-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.25 Arachidonate(s) 0.08 Palmitate(s) 0.5 Cystine(s) 0.16 Oleate(s) 1 Pantothenate(s) 0.43 Stearate(s) 0.08 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-VLDL-PI-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |
| 705 Acyl-CoA-VLDL-PS-pool | Acyl-CoA-VLDL-PS-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-VLDL-PS-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.27 Arachidonate(s) 0.04 Palmitate(s) 0.5 Cystine(s) 0.04 Oleate(s) 1 Pantothenate(s) 0.62 Stearate(s) 0.02 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-VLDL-PS-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 706 Acyl-CoA-VLDL-SM-pool | Acyl-CoA-VLDL-SM-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-VLDL-SM-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.02 Arachidonate(s) 0.71 Palmitate(s) 0.5 Cystine(s) 0.07 Oleate(s) 1 Pantothenate(s) 0.17 Stearate(s) 0.03 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-VLDL-SM-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |
| 707 Acyl-CoA-VLDL-TG2-pool | Acyl-CoA-VLDL-TG2-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-VLDL-TG2-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.06 Arachidonate(s) 0.13 Palmitate(s) 0.5 Cystine(s) 0.46 Oleate(s) 1 Pantothenate(s) 0.04 Stearate(s) 0.31 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-VLDL-TG2-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |
| 708 Acyl-CoA-VLDL-TG3-pool | Acyl-CoA-VLDL-TG3-pool(c) | PIPES MCES | synthesis of cytosolic Acyl-CoA-VLDL-TG3-pool | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.03 Arachidonate(s) 0.09 Palmitate(s) 0.5 Cystine(s) 0.51 Oleate(s) 1 Pantothenate(s) 0.06 Stearate(s) 0.31 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Acyl-CoA-VLDL-TG3-pool(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 48 | - | - | - | - | - | - | - | 15 | - | - | - |
| 709 Adenine | Adenine(s) | PIPES MCES | synthesis of Adenine and blood export | 1 Glycine(s) 2 Asparagine(s) 10 ATP-energy(c) 2 THF-activated methyl group(c) | 1 $CO_2$(s) 2 Pyruvate(c) 1 Adenine(s) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 39 | - | - | - | - | - | - | - | 6 | - | - | - |
| 710 Adenylosuccinate | Adenylosuccinate(c) | PIPES MCES | synthesis of cytosolic Adenylosuccinate | 0.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 7.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 Adenylosuccinate(c) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 2 Na-gradient(c) | 33 | - | - | - | - | - | - | - | 7 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 711 Adenylyl(s)ulfate | Adenylyl sulfate(c) | PIPES MCES | synthesis of cytosolic Adenylyl sulfate | 0.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 10.2 ATP-energy(c) 1 Proton-gradient(c) 1 activated-sulphur(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Adenylyl sulfate(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 2 Na-gradient(c) | 40 | - | - | - | - | - | - | - | 8 | - | - | - |
| 712 Agmatine | Agmatine(m) | PIPES MCES | synthesis of mitochondrial Agmatine | 1 Arginine(s) 1 Proton-gradient(m) | 1 $CO_2$(s) 1 Agmatine(m) | - | 1 | - | - | - | - | - | - | 2 | - | 3 | - |
| 713 Anthranilate | Anthranilate(c) | PIPES MCES | synthesis of cytosolic Anthranilate | 1 $O_2$(s) 1 Tryptophan(s) 1 ATP-energy(c) 2 NADPH-redox-potential(c) | 1 Alanine(s) 1 Anthranilate(c) 1 Na-gradient(c) 1 THF-activated methyl group(c) | 10 | - | - | - | - | - | - | - | 4 | - | - | - |
| 714 Arachidonyl-Carnitine | Arachidonyl-Carnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic Arachidonyl-Carnitine | 1 Arachidonate(s) 1 L-Carnitine(c) 2 ATP-energy(c) | 1 $H_2O$(s) 1 Arachidonyl-Carnitine(c) | 5 | - | - | - | - | - | - | - | 2 | - | - | - |
| 715 Arachidonyl-CoA | Arachidonyl-CoA(c) | PIPES MCES | synthesis of cytosolic Arachidonyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Arachidonate(s) 0.5 Cystine(s) 1 Pantothenate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Arachidonyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 11 | - | - | - |
| 716 Argininosuccinate | Argininosuccinate(c) | PIPES MCES | synthesis of cytosolic Argininosuccinate | 1 Pyruvate(c) 1 Pyruvate(m) 1 Arginine(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 Argininosuccinate(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 4 | 3 | - | - | - | - | - | - | 2 | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 717 But-2-enoyl-ACP | But-2-enoyl-ACP(c) | PIPES MCES | synthesis of cytosolic But-2-enoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 625 ATP-energy(c) 1 NADPH-redox-potential(c) 2 CoA-activated acetyl group(c) | 4 $H_2O$(s) 1 $CO_2$(s) 1 But-2-enoyl-ACP(c) 2 Proton-gradient(c) 82 Na-gradient(c) | 22 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 718 Butyryl-ACP | Butyryl-ACP(c) | PIPES MCES | synthesis of cytosolic Butyryl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 625 ATP-energy(c) 2 NADPH-redox-potential(c) 2 CoA-activated acetyl group(c) | 4 $H_2O$(s) 1 $CO_2$(s) 1 Butyryl-ACP(c) 2 Proton-gradient(c) 82 Na-gradient(c) | 23 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 719 Butyryl-CoA | Butyryl-CoA(c) | PIPES MCES | synthesis of cytosolic Butyryl-CoA | 1.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Butyryl-CoA(c) 7 NADH-redox-potential(m) 5.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 2 Proton-gradient(c) 18 Proton-gradient(m) 5 Na-gradient(c) 7 CoA-activated acetyl group(m) | 43 | 30 | - | - | - | - | - | - | 12 | - | 10 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 720 CDP | CDP(c) | PIPES MCES | synthesis of CDP and blood export | 0.33 $O_2$(s) 1.17 $P_i$(c) 1 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 6.17 ATP-energy(c) | 3.17 $H_2O$(s) 1.33 Glutamate(s) 1 CDP(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 25 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 721 CDP-choline | CDP-choline(c) | PIPES MCES | synthesis of cytosolic CDP-choline | 0.33 $O_2$(s) 1.17 $P_i$(c) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Choline(c) 0.33 Proline(s) 1 Asparagine(s) 8.17 ATP-energy(c) | 4.17 $H_2O$(s) 1.33 Glutamate(s) 1 CDP-choline(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 26 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 722 CDP-ethanolamine | CDP-ethanolamine(c) | PIPES MCES | synthesis of cytosolic CDP-ethanolamine | 0.33 $O_2$(s) 1.17 $P_i$(c) 1 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 1 Ethanolamine(c) 8.17 ATP-energy(c) | 4.17 $H_2O$(s) 1.33 Glutamate(s) 1 CDP-ethanolamine(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 26 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 723 CMP | CMP(c) | PIPES MCES | synthesis of CMP and blood export | 0.33 $O_2$(s) 0.17 $P_i$(c) 1 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 5.17 ATP-energy(c) | 2.17 $H_2O$(s) 1.33 Glutamate(s) 1 CMP(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 26 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 724 CMP-NeuNGc | CMP-NeuNGc(c) | PIPES MCES | synthesis of cytosolic CMP-NeuNGc | 1.33 $O_2$(s) 1 Pyruvate(c) 2 Glutamine(s) 1.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 10.2 ATP-energy(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 3.17 $H_2O$(s) 0.83 $P_i$(c) 2.33 Glutamate(s) 1 CMP-NeuNGc(c) 2 NADH-redox-potential(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 41 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 725 CMP-activated-N-acetylneuraminate | CMP-activated-N-acetylneuraminate(n) | PIPES MCES | synthesis of nucleous CMP-activated-N-acetylneuraminate | 1 Pyruvate(c) 1 Glutamine(s) 1 Glucose-6P(c) 5 ATP-energy(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 1 $P_i$(c) 1 Glutamate(s) 1 NADH-redox-potential(c) 1 CMP-activated-N-acetylneuraminate(n) | 21 | - | - | - | - | 2 | - | - | 2 | - | 4 | - |
| 726 Carbamoyl-P | Carbamoyl-P(c) | PIPES MCES | synthesis of cytosolic Carbamoyl-P | 1 $P_i$(c) 1 Pyruvate(m) 1 Glutamine(s) 2 ATP-energy(c) | 1 Glutamate(s) 1 Carbamoyl-P(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 4 | 3 | - | - | - | - | - | - | 2 | - | 1 | - |
| 727 Carbonate | Carbonate(s) | PIPES MCES | synthesis of Carbonate and blood export | 1 $H_2O$(s) 1 Pyruvate(m) | 1 NADH-redox-potential(m) 1 Carbonate(s) 1 CoA-activated acetyl group(m) | - | 3 | - | - | - | 1 | - | - | 1 | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 728 Carnosine | Carnosine(c) | PIPES MCES | synthesis of cytosolic Carnosine | 1 Aspartate(s) 1 Histidine(s) 2 ATP-energy(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Carnosine(c) 2 Na-gradient(c) | 5 | - | - | - | - | - | - | - | 5 | - | - | - |
| 729 Ceramide-1P-pool | Ceramide-1P-pool(c) | PIPES MCES | synthesis of cytosolic Ceramide-1P-pool | 1 $P_i$(c) 1 Serine(s) 0.02 Arachidonate(s) 0.88 Palmitate(s) 0.24 Oleate(s) 0.03 Linoleate(s) 0.83 Palmitolate(s) 5 ATP-energy(c) 2 NADPH-redox-potential(c) | 3 $H_2O$(s) 1 $CO_2$(s) 1 NADH-redox-potential(c) 1 Proton-gradient(c) 1 Ceramide-1P-pool(c) 1 Na-gradient(c) | 19 | - | - | - | - | - | - | - | 10 | - | - | - |
| 730 Chenodeoxycholoyl-CoA | Chenodeoxycholoyl-CoA(c) | PIPES MCES | synthesis of cytosolic Chenodeoxycholoyl-CoA | 10 $O_2$(s) 0.75 Glycine(s) 1.25 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.25 Proline(s) 0.75 Asparagine(s) 2 Farnesyl-PP(r) 0.88 Cystine(s) 1 Pantothenate(s) 15.2 ATP-energy(c) 11 NADPH-redox-potential(r) 1 NADPH-redox-potential(m) 0.75 Proton-gradient(m) 1.5 THF-activated methyl group(c) | 13.7 $H_2O$(s) 1.83 $P_i$(c) 3.5 $CO_2$(s) 2 Pyruvate(c) 2.25 Glutamate(s) 0.5 Serine(s) 0.75 Methionine(s) 1 Chenodeoxycholoyl-CoA(c) 1 NADH-redox-potential(r) 2.75 NADH-redox-potential(c) 0.13 NADPH-redox-potential(c) 1.5 Proton-gradient(c) 4.5 Na-gradient(c) 0.25 CoA-activated acetyl group(m) | 52 | 12 | 18 | 2 | - | - | - | - | 14 | - | 22 | - |
| 731 Cholate | Cholate(s) | PIPES MCES | synthesis of Cholate and blood export | 11.8 $O_2$(s) 0.5 Cysteine(s) 2 Farnesyl-PP(r) 4 ATP-energy(c) 12 NADPH-redox-potential(r) 2 NADPH-redox-potential(c) 0.5 THF-activated methyl group(c) | 8.5 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 0.5 Pyruvate(c) 0.5 Methionine(s) 1 Cholate(s) 1 NADH-redox-potential(r) 2 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 1 NADH-redox-potential(p) 2.5 Proton-gradient(m) 0.5 Na-gradient(c) 0.5 CoA-activated acetyl group(m) | 15 | 8 | 22 | 6 | - | - | - | - | 9 | - | 23 | - |
| 732 Cholestenol | Cholestenol(r) | PIPES MCES | synthesis of Golgi/ER Cholestenol | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 9 NADPH-redox-potential(r) | 5 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) 1 Cholestenol(r) | 5 | - | 13 | - | - | - | - | - | 3 | - | 5 | - |
| 733 Cholesterol-ester-arach | Cholesterol-ester-arach(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-arach | 8 $O_2$(s) 1 Arachidonate(s) 2 Farnesyl-PP(r) 3 ATP-energy(c) 11 NADPH-redox-potential(r) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-arach(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 8 | - | 18 | - | - | - | - | - | 4 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 734 Cholesterol-ester-gla | Cholesterol-ester-gla(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-gla | 6 $O_2$(s) 1 Arachidonate(s) 2 Farnesyl-PP(r) 3 ATP-energy(c) 7 NADPH-redox-potential(r) | 4 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-gla(r) 1 NADH-redox-potential(r) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 12 | - | 19 | - | - | - | - | - | 4 | - | 8 | - |
| 735 Cholesterol-ester-lin | Cholesterol-ester-lin(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-lin | 5 $O_2$(s) 1 Arachidonate(s) 2 Farnesyl-PP(r) 3 ATP-energy(c) 7 NADPH-redox-potential(r) | 3 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-lin(r) 1 NADH-redox-potential(r) 2 NADH-redox-potential(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 13 | - | 19 | - | - | - | - | - | 4 | - | 10 | - |
| 736 Cholesterol-ester-ol | Cholesterol-ester-ol(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-ol | 8 $O_2$(s) 2 Farnesyl-PP(r) 1 Oleate(s) 3 ATP-energy(c) 11 NADPH-redox-potential(r) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-ol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 6 | - | 18 | - | - | - | - | - | 4 | - | 8 | - |
| 737 Cholesterol-ester-palm | Cholesterol-ester-palm(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-palm | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 Palmitolate(s) 3 ATP-energy(c) 11 NADPH-redox-potential(r) | 6 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-palm(r) 1 NADH-redox-potential(r) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) | 11 | - | 18 | - | - | - | - | - | 4 | - | 6 | - |
| 738 Cholesterol-ester-palmn | Cholesterol-ester-palmn(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-palmn | 8 $O_2$(s) 2 Farnesyl-PP(r) 1 Palmitolate(s) 3 ATP-energy(c) 11 NADPH-redox-potential(r) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-palmn(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 6 | - | 18 | - | - | - | - | - | 4 | - | 8 | - |
| 739 Cholesterol-ester-pool | Cholesterol-ester-pool(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-pool | 6.25 $O_2$(s) 0.59 Arachidonate(s) 2 Farnesyl-PP(r) 0.22 Oleate(s) 0.03 Stearate(s) 0.15 Palmitolate(s) 3 ATP-energy(c) 8.87 NADPH-redox-potential(r) | 5.03 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-pool(r) 1 NADH-redox-potential(r) 1.22 NADH-redox-potential(c) 1 NADPH-redox-potential(c) 0.53 CoA-activated acetyl group(c) | 18 | - | 28 | - | - | - | - | - | 7 | - | 16 | - |
| 740 Cholesterol-ester-stea | Cholesterol-ester-stea(r) | PIPES MCES | synthesis of Golgi/ER Cholesterol-ester-stea | 8 $O_2$(s) 2 Farnesyl-PP(r) 1 Stearate(s) 3 ATP-energy(c) 11 NADPH-redox-potential(r) | 8 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Cholesterol-ester-stea(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 6 | - | 18 | - | - | - | - | - | 4 | - | 8 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 741 Choloyl-CoA | Choloyl-CoA(c) | PIPES MCES | synthesis of cytosolic Choloyl-CoA | 11.5 $O_2$(s) 1 Glycine(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 2 Farnesyl-PP(r) 1 Cystine(s) 1 Pantothenate(s) 16.2 ATP-energy(c) 1 NADH-redox-potential(m) 12 NADPH-redox-potential(r) 1 NADPH-redox-potential(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) | 16.2 $H_2O$(s) 1.83 $P_i$(c) 3 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 Serine(s) 1 Methionine(s) 1 Choloyl-CoA(c) 1 NADH-redox-potential(r) 3 NADH-redox-potential(c) 1 NADH-redox-potential(p) 2 Na-gradient(c) | 53 | 2 | 19 | 7 | - | - | - | - | 9 | - | 18 | - |
| 742 Citrate | Citrate(s) | PIPES MCES | synthesis of Citrate and blood export | 1 $H_2O$(s) 1 Pyruvate(c) 1 Pyruvate(m) 1 NADPH-redox-potential(c) | 1 Citrate(s) 2 NADH-redox-potential(m) 1 Proton-gradient(c) | 2 | 4 | - | - | - | - | - | - | 3 | - | 3 | - |
| 743 Citrulline | Citrulline(s) | PIPES MCES | synthesis of Citrulline and blood export | 0.6 Pyruvate(c) 0.8 Arginine(s) 0.2 Glutamine(s) 0.8 ATP-energy(m) 0.2 NADH-redox-potential(c) 0.4 NADPH-redox-potential(c) 0.2 Proton-gradient(m) | 0.2 Alanine(s) 0.2 Urea(s) 1 Citrulline(s) 0.2 NADH-redox-potential(m) 0.2 NADPH-redox-potential(m) 0.4 CoA-activated acetyl group(m) | 13 | 12 | - | - | - | - | - | - | 4 | - | 6 | - |
| 744 CoproporphyrinogenIII | Coproporphyrinogen[illegible](s) | PIPES MCES | synthesis of cytosolic CoproporphyrinogenIII | 4 Pyruvate(m) 12 Glutamate(s) 4 Serine(s) 4 ATP-energy(c) 4 NADPH-redox-potential(m) 4 Proton-gradient(m) | 12 $H_2O$(s) 12 $CO_2$(s) 4 Aspartate(s) 4 Glutamine(s) 1 CoproporphyrinogenIII(c) 4 NADH-redox-potential(c) 8 NADH-redox-potential(m) 12 Na-gradient(c) | 9 | 8 | - | - | - | - | - | - | 6 | - | 6 | - |
| 745 Crotonyl-CoA | Crotonyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Crotonyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 NADH-redox-potential(m) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Crotonyl-CoA(m) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 42 | 5 | - | - | - | - | - | - | 10 | - | 2 | - |
| 746 Cys-Gly | Cys-Gly(s) | PIPES MCES | synthesis of Cys-Gly and blood export | 1 Glycine(s) 1 Cysteine(s) | 1 $H_2O$(s) 1 Cys-Gly(s) | - | - | - | - | - | - | 1 | - | - | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 747 Cysteamine | Cysteamine(c) | PIPES MCES | synthesis of cytosolic Cysteamine | 1 Cysteine(s) | 1 $CO_2$(s) 1 Cysteamine(c) | 3 | - | - | - | - | - | - | - | 2 | - | - | - |
| 748 D-3-Amino-isobutanoate | D-3-Amino-isobutanoate(s) | PIPES MCES | synthesis of D-3-Amino-isobutanoate and blood export | 0.33 $O_2$(s) 1 Aspartate(s) 0.33 Proline(s) 5 ATP-energy(c) 2 NADH-redox-potential(c) 0.33 Proton-gradient(c) 1 THF-activated methyl group(c) | 1 $CO_2$(s) 0.33 Glutamate(s) 1 D-3-Amino-isobutanoate(s) 0.33 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 4 Proton-gradient(m) 1 Na-gradient(c) | 28 | 4 | - | - | - | - | - | - | 8 | - | 6 | - |
| 749 D-3-Hydroxydodecanoyl-ACP | D-3-Hydroxydodecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic D-3-Hydroxydodecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 629 ATP-energy(c) 9 NADPH-redox-potential(c) 3 Proton-gradient(c) 6 CoA-activated acetyl group(c) | 7 $H_2O$(s) 1 $CO_2$(s) 1 D-3-Hydroxydodecanoyl-ACP(c) 66 Na-gradient(c) | 37 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 750 D-3-Hydroxyhexanoyl-ACP | D-3-Hydroxyhexanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic D-3-Hydroxyhexanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 626 ATP-energy(c) 3 NADPH-redox-potential(c) 3 CoA-activated acetyl group(c) | 4 $H_2O$(s) 1 $CO_2$(s) 1 D-3-Hydroxyhexanoyl-ACP(c) 2 Proton-gradient(c) 82 Na-gradient(c) | 25 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 751 D-Xylulose-5P | D-Xylulose-5P(c) | PIPES MCES | synthesis of cytosolic D-Xylulose-5P | 0.17 $P_i$(c) 0.83 Glucose-6P(c) 0.17 ATP-energy(c) | 0.17 $H_2O$(s) 1 D-Xylulose-5P(c) | 10 | - | - | - | - | - | - | - | 1 | - | - | - |
| 752 DHAP | DHAP(c) | PIPES MCES | synthesis of DHAP and blood export | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.5 ATP-energy(c) | 0.5 $H_2O$(s) 1 DHAP(c) | 5 | - | - | - | - | - | - | - | 1 | - | - | - |
| 753 Deamido-NAD | Deamido-NAD(c) | PIPES MCES | synthesis of cytosolic Deamido-NAD | 0.33 $P_i$(c) 1 Glycine(s) 1 Aspartate(s) 1.67 Glucose-6P(c) 1 Asparagine(s) 1 Nicotinamide(s) 13.3 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.33 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 1 Deamido-NAD(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Na-gradient(c) | 39 | - | - | - | - | - | - | - | 8 | - | - | - |
| 754 Decanoyl-ACP | Decanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic Decanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 628 ATP-energy(c) 8 NADPH-redox-potential(c) 3 Proton-gradient(c) 5 CoA-activated acetyl group(c) | 7 $H_2O$(s) 1 $CO_2$(s) 1 Decanoyl-ACP(c) 66 Na-gradient(c) | 35 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 755 Decanoyl-CoA | Decanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Decanoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Decanoyl-CoA(m) 2 NADH-redox-potential(c) 4 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 3 Na-gradient(c) 4 CoA-activated acetyl group(m) | 44 | 18 | - | - | - | - | - | - | 11 | - | 3 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 756 Dehydroalanine | Dehydroalanine(c) | PIPES MCES | synthesis of cytosolic Dehydroalanine | 1 Serine(s) | 1 $H_2O$(s) 1 Dehydroalanine(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 1 | - | - | - | - | - | - | - | 4 | - | - | - |
| 757 Deoxyadenosine | Deoxyadenosine(s) | PIPES MCES | synthesis of Deoxyadenosine and blood export | 1 Glycine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 9.17 ATP-energy(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 0.83 $P_i$(c) 1 $CO_2$(s) 2 Pyruvate(c) 1 Deoxyadenosine(s) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 40 | - | - | - | - | - | - | - | 7 | - | - | - |
| 758 Deoxycytidine | Deoxycytidine(s) | PIPES MCES | synthesis of Deoxycytidine and blood export | 0.33 $O_2$(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 6.17 ATP-energy(c) 1 NADPH-redox-potential(c) | 2.17 $H_2O$(s) 0.83 $P_i$(c) 1.33 Glutamate(s) 1 Deoxycytidine(s) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 30 | 4 | - | - | - | - | - | - | 8 | - | 6 | - |
| 759 Deoxyguanosine | Deoxyguanosine(s) | PIPES MCES | synthesis of Deoxyguanosine and blood export | 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 8.17 ATP-energy(c) 2 THF-activated methyl group(c) | 0.17 $H_2O$(s) 0.83 $P_i$(c) 1 Pyruvate(c) 2 Glutamate(s) 1 Deoxyguanosine(s) 3 NADH-redox-potential(c) 2 NADPH-redox-potential(c) | 39 | - | - | - | - | - | - | - | 6 | - | - | - |
| 760 Deoxyinosine | Deoxyinosine(s) | PIPES MCES | synthesis of Deoxyinosine and blood export | 1 Glycine(s) 1 Aspartate(s) 1 Glutamine(s) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 8.5 ATP-energy(c) 2 THF-activated methyl group(c) | 1.5 $H_2O$(s) 0.5 $P_i$(c) 1 Pyruvate(c) 1 Glutamate(s) 1 Deoxyinosine(s) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Na-gradient(c) | 35 | - | - | - | - | - | - | - | 7 | - | - | - |
| 761 Deoxyuridine | Deoxyuridine(s) | PIPES MCES | synthesis of Deoxyuridine and blood export | 0.33 $O_2$(s) 1 Aspartate(s) 0.5 Glucose-6P(c) 0.33 Proline(s) 1 Ethanolamine(c) 5.5 ATP-energy(c) | 2.5 $H_2O$(s) 0.5 $P_i$(c) 0.33 Glutamate(s) 1 Deoxyuridine(s) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 24 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 762 Dephospho-CoA | Dephospho-CoA(c) | PIPES MCES | synthesis of cytosolic Dephospho-CoA | 1.17 $P_i$(c) 1 Glycine(s) 0.5 Aspartate(s) 0.5 Glutamine(s) 0.83 Glucose-6P(c) 1.5 Asparagine(s) 0.5 Cystine(s) 1 Pantothenate(s) 11.7 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 Dephospho-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1.5 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 10 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 763 Desmosterol | Desmosterol(r) | PIPES MCES | synthesis of Golgi/ER Desmosterol | 8 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 10 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Desmosterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 15 | - | - | - | - | - | 3 | - | 5 | - |
| 764 Dihomo-gamma-linolenoyl-CoA | Dihomo-gamma-linolenoyl-CoA(c) | PIPES MCES | synthesis of cytosolic Dihomo-gamma-linolenoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 1 Phenylalanine(s) 0.83 Glucose-6P(c) 1 Arachidonate(s) 0.5 Cystine(s) 1 Pantothenate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Tyrosine(s) 1 Dihomo-gamma-linolenoyl-CoA(c) 3 NADH-redox-potential(c) 2.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 46 | - | - | - | - | - | - | - | 11 | - | - | - |
| 765 Dihydroceramide-pool | Dihydroceramide-pool(c) | PIPES MCES | synthesis of cytosolic Dihydroceramide-pool | 1 Serine(s) 0.02 Arachidonate(s) 1.71 Palmitate(s) 0.07 Oleate(s) 0.17 Stearate(s) 0.03 Linoleate(s) 4 ATP-energy(c) 1 NADPH-redox-potential(c) | 2 $H_2O$(s) 1 $CO_2$(s) 1 Proton-gradient(c) 1 Dihydroceramide-pool(c) 1 Na-gradient(c) | 13 | - | - | - | - | - | - | - | 10 | - | - | - |
| 766 Dihydrofolate | Dihydrofolate(c) | PIPES MCES | synthesis of cytosolic Dihydrofolate | 1 Folate(s) 1 NADPH-redox-potential(c) | 1 Dihydrofolate(c) | 2 | - | - | - | - | - | - | - | 1 | - | - | - |
| 767 Dihydrothymine | Dihydrothymine(c) | PIPES MCES | synthesis of cytosolic Dihydrothymine | 0.33 $O_2$(s) 1 Aspartate(s) 1 Glutamine(s) 0.33 Proline(s) 4 ATP-energy(c) 1 NADH-redox-potential(c) 1 THF-activated methyl group(c) | 1 $H_2O$(s) 1.33 Glutamate(s) 1 Dihydrothymine(c) 0.33 NADH-redox-potential(m) 1 Proton-gradient(c) 4 Proton-gradient(m) 2.33 Na-gradient(c) | 24 | 4 | - | - | - | - | - | - | 8 | - | 6 | - |
| 768 Dimethylallyl-PP | Dimethylallyl-PP(p) | PIPES MCES | synthesis of peroxysomal Dimethylallyl-PP | 2 $P_i$(c) 3 ATP-energy(c) 2 NADPH-redox-potential(c) 3 CoA-activated acetyl group(c) | 2 $H_2O$(s) 1 $CO_2$(s) 1 Dimethylallyl-PP(p) | 6 | - | - | 4 | - | - | - | - | 2 | - | 4 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 769 Dodecanoyl-ACP | Dodecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic Dodecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 629 ATP-energy(c) 10 NADPH-redox-potential(c) 3 Proton-gradient(c) 6 CoA-activated acetyl group(c) | 8 $H_2O$(s) 1 $CO_2$(s) 1 Dodecanoyl-ACP(c) 66 Na-gradient(c) | 39 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 770 Erythrose-4P | Erythrose-4P(c) | PIPES MCES | synthesis of cytosolic Erythrose-4P | 0.33 $P_i$(c) 0.67 Glucose-6P(c) 0.33 ATP-energy(c) | 0.33 $H_2O$(s) 1 Erythrose-4P(c) | 9 | - | - | - | - | - | - | - | 1 | - | - | - |
| 771 Ethanolamine-P | Ethanolamine-P(c) | PIPES MCES | synthesis of cytosolic Ethanolamine-P | 1 $P_i$(c) 1 Ethanolamine(c) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Ethanolamine-P(c) | 2 | - | - | - | - | - | - | - | 1 | - | - | - |
| 772 FADH2 | FADH2(c) | PIPES MCES | synthesis of cytosolic FADH2 | 1.17 $P_i$(c) 1 Glycine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 1 Riboflavin(s) 12.2 ATP-energy(c) 1 FADH-redox-potential(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 1 FADH2(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) | 39 | - | - | - | - | - | - | - | 6 | - | - | - |
| 773 FAICAR | FAICAR(c) | PIPES MCES | synthesis of cytosolic FAICAR | 0.17 $P_i$(c) 1 Glycine(s) 1 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 6.17 ATP-energy(c) 2 THF-activated methyl group(c) | 0.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 FAICAR(c) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Proton-gradient(c) 3 Na-gradient(c) | 30 | - | - | - | - | - | - | - | 7 | - | - | - |
| 774 FMN | FMN(c) | PIPES MCES | synthesis of cytosolic FMN | 1 $P_i$(c) 1 Riboflavin(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 FMN(c) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 775 Fatty-acid-VLDL-PC-pool | Fatty-acid-VLDL-PC-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-PC-pool | 0.08 Arachidonate(s) 0.35 Palmitate(s) 0.14 Oleate(s) 0.15 Stearate(s) 0.27 Linoleate(s) | 1 Fatty-acid-VLDL-PC-pool(c) | 1 | - | - | - | - | - | - | - | 5 | - | - | - |
| 776 Fatty-acid-VLDL-PE-pool | Fatty-acid-VLDL-PE-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-PE-pool | 0.3 Arachidonate(s) 0.17 Palmitate(s) 0.08 Oleate(s) 0.27 Stearate(s) 0.18 Linoleate(s) 2.5 ATP-energy(c) | 1 Fatty-acid-VLDL-PE-pool(c) | 20 | - | - | - | - | - | - | - | 5 | - | - | - |
| 777 Fatty-acid-VLDL-PI-pool | Fatty-acid-VLDL-PI-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-PI-pool | 0.25 Arachidonate(s) 0.08 Palmitate(s) 0.16 Oleate(s) 0.43 Stearate(s) 0.08 Linoleate(s) 2.5 ATP-energy(c) | 1 Fatty-acid-VLDL-PI-pool(c) | 20 | - | - | - | - | - | - | - | 5 | - | - | - |
| 778 Fatty-acid-VLDL-PS-pool | Fatty-acid-VLDL-PS-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-PS-pool | 0.27 Arachidonate(s) 0.04 Palmitate(s) 0.04 Oleate(s) 0.62 Stearate(s) 0.02 Linoleate(s) 2.5 ATP-energy(c) | 1 Fatty-acid-VLDL-PS-pool(c) | 20 | - | - | - | - | - | - | - | 5 | - | - | - |
| 779 Fatty-acid-VLDL-SM-pool | Fatty-acid-VLDL-SM-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-SM-pool | 0.02 Arachidonate(s) 0.71 Palmitate(s) 0.07 Oleate(s) 0.17 Stearate(s) 0.03 Linoleate(s) | 1 Fatty-acid-VLDL-SM-pool(c) | 1 | - | - | - | - | - | - | - | 5 | - | - | - |
| 780 Fatty-acid-VLDL-TG1-pool | Fatty-acid-VLDL-TG1-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-TG1-pool | 0.003 Arachidonate(s) 0.7 Palmitate(s) 0.13 Oleate(s) 0.09 Stearate(s) 0.08 Linoleate(s) 5 ATP-energy(c) | 1 Fatty-acid-VLDL-TG1-pool(c) | 21 | - | - | - | - | - | - | - | 5 | - | - | - |
| 781 Fatty-acid-VLDL-TG2-pool | Fatty-acid-VLDL-TG2-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-TG2-pool | 0.06 Arachidonate(s) 0.13 Palmitate(s) 0.46 Oleate(s) 0.04 Stearate(s) 0.31 Linoleate(s) 5 ATP-energy(c) | 1 Fatty-acid-VLDL-TG2-pool(c) | 21 | - | - | - | - | - | - | - | 5 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 782 Fatty-acid-VLDL-TG3-pool | Fatty-acid-VLDL-TG3-pool(c) | PIPES MCES | synthesis of cytosolic Fatty-acid-VLDL-TG3-pool | 0.03 Arachidonate(s) 0.09 Palmitate(s) 0.51 Oleate(s) 0.06 Stearate(s) 0.31 Linoleate(s) 2 ATP-energy(c) | 1 Fatty-acid-VLDL-TG3-pool(c) | 11 | - | - | - | - | - | - | - | 5 | - | - | - |
| 783 Formamidopyrimidine(f) nucleoside triphosphate | Formamidopyrimidine(f) nucleoside triphosphate(c) | PIPES MCES | synthesis of cytosolic Formamidopyrimidine nleoside triphosphate | 2.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 10.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 Formamidopyrimidine nleoside triphosphate(c) 3 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 37 | - | - | - | - | - | - | - | 6 | - | - | - |
| 784 Formylanthranilate | Formylanthranilate(c) | PIPES MCES | synthesis of cytosolic Formylanthranilate | 1 $H_2O$(s) 1 $O_2$(s) 1 Tryptophan(s) | 1 Alanine(s) 1 Formylanthranilate(c) 2 Na-gradient(c) | 2 | - | - | - | - | - | - | - | 5 | - | - | - |
| 785 Fructose-1,6PP | Fructose-1,6PP(c) | PIPES MCES | synthesis of cytosolic Fructose-1,6PP | 1 $P_i$(c) 1 Glucose-6P(c) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Fructose-1,6PP(c) | 3 | - | - | - | - | - | - | - | 1 | - | - | - |
| 786 Fructose-2,6PP | Fructose-2,6PP(c) | PIPES MCES | synthesis of cytosolic Fructose-2,6PP | 1 $P_i$(c) 1 Glucose-6P(c) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Fructose-2,6PP(c) | 3 | - | - | - | - | - | - | - | 1 | - | - | - |
| 787 Fumarate | Fumarate(c) | PIPES MCES | synthesis of cytosolic Fumarate | 1 Pyruvate(c) 1 Pyruvate(m) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 Fumarate(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 3 | 3 | - | - | - | - | - | - | 1 | - | 1 | - |
| 788 Fumarylacetoacetate | Fumarylacetoacetate(c) | PIPES MCES | synthesis of cytosolic Fumarylacetoacetate | 2 $O_2$(s) 1 Pyruvate(c) 1 Tyrosine(s) | 1 $CO_2$(s) 1 Alanine(s) 1 Fumarylacetoacetate(c) 1 Na-gradient(c) | 5 | - | - | - | - | - | - | - | 5 | - | - | - |
| 789 GAP | GAP(c) | PIPES MCES | synthesis of cytosolic GAP | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.5 ATP-energy(c) | 0.5 $H_2O$(s) 1 GAP(c) | 5 | - | - | - | - | - | - | - | 1 | - | - | - |
| 790 GAR | GAR(c) | PIPES MCES | synthesis of cytosolic GAR | 0.17 $P_i$(c) 1 Glycine(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 3.17 ATP-energy(c) 1 Proton-gradient(c) | 1.17 $H_2O$(s) 1 Glutamate(s) 1 GAR(c) | 15 | - | - | - | - | - | - | - | 5 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 791 GDP | GDP(c) | PIPES MCES | synthesis of GDP | 1.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 9.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 GDP(c) 3 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 35 | - | - | - | - | - | - | - | 6 | - | - | - |
| 792 GMP | GMP(c) | PIPES MCES | synthesis of GMP | 0.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 8.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 0.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 GMP(c) 3 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 34 | - | - | - | - | - | - | - | 6 | - | - | - |
| 793 GSSG | GSSG(c) | PIPES MCES | synthesis of GSSG | 2 Glutamate(s) 2 Glycine(s) 2 Cysteine(s) 4 ATP-energy(c) 2 Proton-gradient(c) | 4 $H_2O$(s) 1 GSSG(c) 1 NADPH-redox-potential(c) 2 Na-gradient(c) | 5 | - | - | - | - | - | - | - | 6 | - | - | - |
| 794 Galactose-1P | Galactose-1P(c) | PIPES MCES | synthesis of cytosolic Galactose-1P | 1 Glucose-6P(c) | 1 Galactose-1P(c) | 3 | - | - | - | - | - | - | - | - | - | - | - |
| 795 Geranyl-PP | Geranyl-PP(p) | PIPES MCES | synthesis of peroxysomal Geranyl-PP | 2 $P_i$(c) 6 ATP-energy(c) 4 NADPH-redox-potential(c) 6 CoA-activated acetyl group(c) | 3 $H_2O$(s) 2 $CO_2$(s) 1 Geranyl-PP(p) | 7 | - | - | 5 | - | - | - | - | 2 | - | 5 | - |
| 796 Glucono-1,5-lactone-6P | Glucono-1,5-lactone-6P(c) | PIPES MCES | synthesis of cytosolic Glucono-1,5-lactone-6P | 1 Glucose-6P(c) | 1 Glucono-1,5-lactone-6P(c) 1 NADPH-redox-potential(c) | 2 | - | - | - | - | - | - | - | - | - | - | - |
| 797 Glucose-1P | Glucose-1P(c) | PIPES MCES | synthesis of Glucose-1P | 1 Glucose-6P(c) | 1 Glucose-1P(c) | 1 | - | - | - | - | - | - | - | - | - | - | - |
| 798 Glucosylceramide-pool | Glucosylceramide-pool(c) | PIPES MCES | synthesis of Glucosylceramide-pool | 1 Serine(s) 1 Glucose-6P(c) 0.02 Arachidonate(s) 0.88 Palmitate(s) 0.24 Oleate(s) 0.03 Linoleate(s) 0.83 Palmitolate(s) 5 ATP-energy(c) 2 NADPH-redox-potential(c) | 2 $H_2O$(s) 1 $P_i$(c) 1 $CO_2$(s) 1 Glucosylceramide-pool(c) 1 NADH-redox-potential(c) | 22 | - | - | - | - | - | - | - | 8 | - | - | - |
| 799 Glucuronate | Glucuronate(c) | PIPES MCES | synthesis of cytosolic Glucuronate | 1 $O_2$(s) 1 Glucose-6P(c) | 1 $P_i$(c) 1 Glucuronate(c) | 3 | - | - | - | - | - | - | - | 1 | - | - | - |
| 800 Glutamyl-5P | Glutamyl-5P(m) | PIPES MCES | synthesis of mitochondrial Glutamyl-5P | 1 $P_i$(c) 0.5 Glutamate(s) 0.5 Proline(s) 1 ATP-energy(m) | 1 Glutamyl-5P(m) 1 Na-gradient(c) | - | 5 | - | - | - | - | - | - | 3 | - | 4 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 801 Glutaryl-CoA | Glutaryl-CoA(m) | PIPES MCES | synthesis of mitochondrial Glutaryl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 2 NADH-redox-potential(m) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 2 CoA-activated acetyl group(m) | 6.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Glutaryl-CoA(m) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 4 Proton-gradient(m) 3 Na-gradient(c) | 42 | 6 | - | - | - | - | - | - | 10 | - | 5 | - |
| 802 Glycerate | Glycerate(c) | PIPES MCES | synthesis of cytosolic Glycerate | 1 Pyruvate(c) 1 Serine(s) 1 NADPH-redox-potential(c) | 1 Alanine(s) 1 Glycerate(c) 2 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 3 | - | - | - |
| 803 Glycogenin-G11 | Glycogenin-G11(c) | PIPES MCES | synthesis of cytosolic Glycogenin-G11 | 15 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 18 Lysine(s) 26 Aspartate(s) 12 Arginine(s) 14 Glutamine(s) 31 Serine(s) 8 Methionine(s) 7 Tryptophan(s) 20 Phenylalanine(s) 13 Tyrosine(s) 11 Glucose-6P(c) 6 Cysteine(s) 39 Leucine(s) 9 Histidine(s) 15 Proline(s) 12 Asparagine(s) 28 Valine(s) 25 Threonine(s) 12 Isoleucine(s) 1761 ATP-energy(c) | 11 $P_i$(c) 3 Proton-gradient(c) 1 Glycogenin-G11(c) 246 Na-gradient(c) | 8 | - | - | - | - | - | - | - | 22 | - | - | 1 |
| 804 Glycogenin-G4G4 | Glycogenin-G4G4(c) | PIPES MCES | synthesis of cytosolic Glycogenin-G4G4 | 15 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 18 Lysine(s) 26 Aspartate(s) 12 Arginine(s) 14 Glutamine(s) 31 Serine(s) 8 Methionine(s) 7 Tryptophan(s) 20 Phenylalanine(s) 13 Tyrosine(s) 8 Glucose-6P(c) 6 Cysteine(s) 39 Leucine(s) 9 Histidine(s) 15 Proline(s) 12 Asparagine(s) 28 Valine(s) 25 Threonine(s) 12 Isoleucine(s) 1761 ATP-energy(c) | 8 $P_i$(c) 3 Proton-gradient(c) 1 Glycogenin-G4G4(c) 246 Na-gradient(c) | 10 | - | - | - | - | - | - | - | 22 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 805 Glycogenin-G7 | Glycogenin-G7(c) | PIPES MCES | synthesis of cytosolic Glycogenin-G7 | 15 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 18 Lysine(s) 26 Aspartate(s) 12 Arginine(s) 14 Glutamine(s) 31 Serine(s) 8 Methionine(s) 7 Tryptophan(s) 20 Phenylalanine(s) 13 Tyrosine(s) 7 Glucose-6P(c) 6 Cysteine(s) 39 Leucine(s) 9 Histidine(s) 15 Proline(s) 12 Asparagine(s) 28 Valine(s) 25 Threonine(s) 12 Isoleucine(s) 1762 ATP-energy(c) | 7 $P_i$(c) 3 Proton-gradient(c) 1 Glycogenin-G7(c) 246 Na-gradient(c) | 13 | - | - | - | - | - | - | - | 22 | - | - | 1 |
| 806 Glycogenin-G7G1 | Glycogenin-G7G1(c) | PIPES MCES | synthesis of cytosolic Glycogenin-G7G1 | 15 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 18 Lysine(s) 26 Aspartate(s) 12 Arginine(s) 14 Glutamine(s) 31 Serine(s) 8 Methionine(s) 7 Tryptophan(s) 20 Phenylalanine(s) 13 Tyrosine(s) 8 Glucose-6P(c) 6 Cysteine(s) 39 Leucine(s) 9 Histidine(s) 15 Proline(s) 12 Asparagine(s) 28 Valine(s) 25 Threonine(s) 12 Isoleucine(s) 1761 ATP-energy(c) | 8 $P_i$(c) 3 Proton-gradient(c) 1 Glycogenin-G7G1(c) 246 Na-gradient(c) | 11 | - | - | - | - | - | - | - | 22 | - | - | 1 |
| 807 Glycogenin-G8 | Glycogenin-G8(c) | PIPES MCES | synthesis of cytosolic Glycogenin-G8 | 15 Glutamate(s) 18 Glycine(s) 22 Alanine(s) 18 Lysine(s) 26 Aspartate(s) 12 Arginine(s) 14 Glutamine(s) 31 Serine(s) 8 Methionine(s) 7 Tryptophan(s) 20 Phenylalanine(s) 13 Tyrosine(s) 8 Glucose-6P(c) 6 Cysteine(s) 39 Leucine(s) 9 Histidine(s) 15 Proline(s) 12 Asparagine(s) 28 Valine(s) 25 Threonine(s) 12 Isoleucine(s) 1758 ATP-energy(c) | 8 $P_i$(c) 3 Proton-gradient(c) 1 Glycogenin-G8(c) 246 Na-gradient(c) | 7 | - | - | - | - | - | - | - | 22 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 808 Guanidinoacetate | Guanidinoacetate(c) | PIPES MCES | synthesis of cytosolic Guanidinoacetate | 0.08 $O_2$(s) 1 Glycine(s) 0.5 Aspartate(s) 0.5 Arginine(s) 1 ATP-energy(c) 1 ATP-energy(m) 0.83 Proton-gradient(c) | 0.5 Pyruvate(c) 0.33 Glutamate(s) 0.17 Proline(s) 1 Guanidinoacetate(c) 0.33 NADH-redox-potential(m) 0.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) 0.67 Na-gradient(c) | 9 | 10 | - | - | - | - | - | - | 8 | - | 9 | - |
| 809 Guanosine | Guanosine(s) | PIPES MCES | synthesis of Guanosine and blood export | 0.17 Glycine(s) 2 Glutamine(s) 0.83 Serine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 8.17 ATP-energy(c) 1.17 THF-activated methyl group(c) | 0.83 $P_i$(c) 1 Pyruvate(c) 2 Glutamate(s) 1 Guanosine(s) 2.17 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 2.83 Proton-gradient(c) 2.83 Na-gradient(c) | 36 | - | - | - | - | - | - | - | 8 | - | - | - |
| 810 $H_2O_2$ | $H_2O_2$(c) | PIPES MCES | synthesis of $H_2O_2$ and blood export | 1 $O_2$(s) 1 $NH_3$(s) 1 Aspartate(s) 1 Glutamine(s) 1 Serine(s) 8 ATP-energy(c) 1 THF-activated methyl group(c) | 1 Pyruvate(c) 1 Glutamate(s) 1 $H_2O_2$(c) 1 Urate(s) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 29 | - | - | - | - | - | - | - | 9 | - | - | - |
| 811 $H_2S$ | $H_2S$(s) | PIPES MCES | synthesis of $H_2S$ and blood export | 1 Glutamate(s) 1 Cysteine(s) 1 ATP-energy(c) | 1 Pyruvate(c) 1 Glutamine(s) 1 $H_2S$(s) 1 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 5 | - | - | - |
| 812 HCO3- | HCO3-(s) | PIPES MCES | synthesis of HCO3- and blood export | 1 $H_2O$(s) 1 Pyruvate(m) | 1 HCO3-(s) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | - | 3 | - | - | - | - | 2 | - | 1 | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 813 HMA | HMA(c) | PIPES MCES | synthesis of cytosolic HMA | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 630 ATP-energy(c) 11 NADPH-redox-potential(c) 3 Proton-gradient(c) 7 CoA-activated acetyl group(c) | 8 $H_2O$(s) 1 $CO_2$(s) 1 HMA(c) 66 Na-gradient(c) | 41 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 814 HMG-CoA | HMG-CoA(c) | PIPES MCES | synthesis of cytosolic HMG-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 3 CoA-activated acetyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 HMG-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 45 | - | - | - | - | - | - | - | 10 | - | - | - |
| 815 Hexadecanal | Hexadecanal(c) | PIPES MCES | synthesis of cytosolic Hexadecanal | 1 Serine(s) 1 Palmitolate(s) 3 ATP-energy(c) 3 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Ethanolamine(c) 1 Hexadecanal(c) 1 NADH-redox-potential(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 17 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 816 Hexadecanoyl-ACP | Hexadecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic Hexadecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 631 ATP-energy(c) 14 NADPH-redox-potential(c) 3 Proton-gradient(c) 8 CoA-activated acetyl group(c) | 10 $H_2O$(s) 1 $CO_2$(s) 1 Hexadecanoyl-ACP(c) 66 Na-gradient(c) | 47 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 817 Hexadecenal | Hexadecenal(c) | PIPES MCES | synthesis of cytosolic Hexadecenal | 1 Serine(s) 1 Palmitolate(s) 3 ATP-energy(c) 2 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Ethanolamine(c) 1 NADH-redox-potential(c) 1 Proton-gradient(c) 1 Hexadecenal(c) 1 Na-gradient(c) | 16 | - | - | - | - | - | - | - | 6 | - | - | - |
| 818 Hexanoyl-ACP | Hexanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic Hexanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 626 ATP-energy(c) 4 NADPH-redox-potential(c) 3 Proton-gradient(c) 3 CoA-activated acetyl group(c) | 5 $H_2O$(s) 1 $CO_2$(s) 1 Hexanoyl-ACP(c) 66 Na-gradient(c) | 27 | - | - | - | - | - | - | - | 24 | - | - | 1 |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 819 Hexanoyl-CoA | Hexanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Hexanoyl-CoA | 1 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Hexanoyl-CoA(m) 2 NADH-redox-potential(c) 6 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 12 Proton-gradient(m) 3 Na-gradient(c) 6 CoA-activated acetyl group(m) | 44 | 26 | - | - | - | - | - | - | 12 | - | 7 | - |
| 820 Histamine | Histamine(s) | PIPES MCES | synthesis of Histamine and blood export | 1 Histidine(s) | 1 $CO_2$(s) 1 Histamine(s) 1 Na-gradient(c) | 1 | - | - | - | - | - | - | - | 4 | - | - | - |
| 821 Homogentisate | Homogentisate(c) | PIPES MCES | synthesis of cytosolic Homogentisate | 1 $O_2$(s) 1 Pyruvate(c) 1 Tyrosine(s) | 1 $CO_2$(s) 1 Alanine(s) 1 Homogentisate(c) 1 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 5 | - | - | - |
| 822 Homovanillate | Homovanillate(m) | PIPES MCES -3-Methoxy-4-hydroxyphenylacetaldehyde(m) | synthesis of mitochondrial Homovanillate using 3-Methoxy-4-hydroxyphenylacetaldehyde | 1 $H_2O$(s) 1 3-Methoxy-4-hydroxyphenylacetaldehyde(m) | 1 Homovanillate(m) 1 NADH-redox-potential(m) | - | 2 | - | - | - | - | - | - | 1 | - | 1 | - |
| 823 Hydracrylate | Hydracrylate(m) | PIPES MCES | synthesis of mitochondrial Hydracrylate | 0.5 $O_2$(s) 1 Glutamate(s) 1 Threonine(s) 1 ATP-energy(c) | 1 $CO_2$(s) 1 Glutamine(s) 1 Hydracrylate(m) 1 NADH-redox-potential(m) 5 Proton-gradient(m) 2 Na-gradient(c) | 3 | 5 | - | - | - | - | - | - | 6 | - | 7 | - |
| 824 Hydroxymethylbilane | Hydroxymethylbilane(c) | PIPES MCES | synthesis of cytosolic Hydroxymethylbilane | 4 Pyruvate(m) 12 Glutamate(s) 4 Serine(s) 4 ATP-energy(c) 4 NADPH-redox-potential(m) 4 Proton-gradient(m) | 11 $H_2O$(s) 8 $CO_2$(s) 4 Aspartate(s) 4 Glutamine(s) 1 Hydroxymethylbilane(c) 4 NADH-redox-potential(c) 8 NADH-redox-potential(m) 12 Na-gradient(c) | 7 | 8 | - | - | - | - | - | - | 6 | - | 6 | - |
| 825 Hydroxypyruvate | Hydroxypyruvate(c) | Pyruvate(c) −Serine(c) +Alanine(c) | synthesis of cytosolic Hydroxypyruvate | 1 Pyruvate(c) 1 Serine(c) | 1 Alanine(c) 1 Hydroxypyruvate(c) | 1 | - | - | - | - | - | - | - | - | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 826 Hypotaurine | Hypotaurine(c) | PIPES MCES | synthesis of cytosolic Hypotaurine | 1 $O_2$(s) 1 Cysteine(s) | 1 $CO_2$(s) 1 Hypotaurine(c) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 827 Hypoxanthine | Hypoxanthine(s) | PIPES MCES | synthesis of Hypoxanthine and blood export | 1 Glycine(s) 1 Glutamine(s) 1 Asparagine(s) 7 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1 Pyruvate(c) 1 Glutamate(s) 1 Hypoxanthine(s) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 27 | - | - | - | - | - | - | - | 6 | - | - | - |
| 828 Inosine | Inosine(s) | PIPES MCES | synthesis of Inosine and blood export | 1 Glycine(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 7.17 ATP-energy(c) 2 THF-activated methyl group(c) | 0.17 $H_2O$(s) 0.83 $P_i$(c) 1 Pyruvate(c) 1 Glutamate(s) 1 Inosine(s) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Na-gradient(c) | 34 | - | - | - | - | - | - | - | 7 | - | - | - |
| 829 Inositol | Inositol(s) | PIPES MCES | synthesis of Inositol and blood export | 1 $H_2O$(s) 1 Glucose-6P(c) | 1 $P_i$(c) 1 Inositol(s) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |
| 830 Inositol-1P | Inositol-1P(c) | PIPES MCES | synthesis of cytosolic Inositol-1P | 1 Glucose-6P(c) | 1 Inositol-1P(c) | 1 | - | - | - | - | - | - | - | - | - | - | - |
| 831 Isobutyryl-CoA | Isobutyryl-CoA(m) | PIPES MCES | synthesis of mitochondrial Isobutyryl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Valine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 1 Proton-gradient(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 Isobutyryl-CoA(m) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 4 Na-gradient(c) | 43 | 5 | - | - | - | - | - | - | 11 | - | 6 | - |
| 832 Isocitrate | Isocitrate(c) | PIPES MCES | synthesis of cytosolic Isocitrate | 1 Pyruvate(c) 1 Pyruvate(m) 1 Glutamate(s) 1 NADPH-redox-potential(c) | 1 Alanine(s) 1 Isocitrate(c) 1 NADH-redox-potential(m) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 4 | 3 | - | - | - | - | - | - | 3 | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 833 Isovaleryl-CoA | Isovaleryl-CoA(m) | PIPES MCES | synthesis of mitochondrial Isovaleryl-CoA | 2.17 $P_i$(c) 0.25 Pyruvate(m) 1 Glycine(s) 1.75 Aspartate(s) 1.5 Glutamine(s) 0.83 Glucose-6P(c) 0.75 Leucine(s) 0.5 Cystine(s) 1 Pantothenate(s) 11.7 ATP-energy(c) 1.25 Proton-gradient(m) 2 THF-activated methyl group(c) 0.75 CoA-activated acetyl group(m) | 5.67 $H_2O$(s) 2.75 $CO_2$(s) 2 Pyruvate(c) 1.25 Glutamate(s) 0.25 Proline(s) 1 Isovaleryl-CoA(m) 2 NADH-redox-potential(c) 0.5 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 0.5 NADPH-redox-potential(m) 3.75 Na-gradient(c) | 43 | 16 | - | - | - | - | - | - | 11 | - | 7 | - |
| 834 Kynurenine | Kynurenine(c) | PIPES MCES | synthesis of cytosolic Kynurenine | 1 $O_2$(s) 1 Tryptophan(s) 1 ATP-energy(c) 0.5 NADPH-redox-potential(c) | 0.5 $CO_2$(s) 1 Kynurenine(c) 1 Na-gradient(c) 0.5 THF-activated methyl group(c) | 10 | - | - | - | - | - | - | - | 4 | - | - | - |
| 835 L-1-Pyrroline-3-hydroxy-5-carboxylate | L-1-Pyrroline-3-hydroxy-5-carboxylate(c) | PIPES MCES −trans-4-Hydroxy-L-proline(c) | synthesis of cytosolic L-1-Pyrroline-3-hydroxy-5-carboxylate | 1 trans-4-Hydroxy-L-proline(c) | 1 L-1-Pyrroline-3-hydroxy-5-carboxylate(c) 1 NADPH-redox-potential(c) | 2 | - | - | - | - | - | - | - | - | - | - | - |
| 836 L-2-Aminoadipate | L-2-Aminoadipate(c) | PIPES MCES -2-Aminoadipate 6-semialdehyde(c) | synthesis of cytosolic L-2-Aminoadipate | 1 $H_2O$(s) 1 2-Aminoadipate 6-semialdehyde(c) | 1 L-2-Aminoadipate(c) 1 NADH-redox-potential(c) | 2 | - | - | - | - | - | - | - | 1 | - | - | - |
| 837 L-Cystathionine | L-Cystathionine(c) | PIPES MCES | synthesis of cytosolic L-Cystathionine | 1 Serine(s) 1 Methionine(s) | 1 $H_2O$(s) 1 L-Cystathionine(c) 1 Proton-gradient(c) 2 Na-gradient(c) 1 THF-activated methyl group(c) | 3 | - | - | - | - | - | - | - | 5 | - | - | - |
| 838 L-Formylkynurenine | L-Formylkynurenine(c) | PIPES MCES | synthesis of cytosolic L-Formylkynurenine | 1 $O_2$(s) 1 Tryptophan(s) | 1 L-Formylkynurenine(c) 1 Na-gradient(c) | 1 | - | - | - | - | - | - | - | 3 | - | - | - |
| 839 L-Fucose-1P | L-Fucose-1P(c) | PIPES MCES | synthesis of cytosolic L-Fucose-1P | 1 Glucose-6P(c) 1 NADH-redox-potential(c) | 1 $H_2O$(s) 1 L-Fucose-1P(c) | 8 | - | - | - | - | - | - | - | 1 | - | - | - |
| 840 L-Glutamate 5-semialdehyde | L-Glutamate 5-semialdehyde(m) | PIPES MCES | synthesis of mitochondrial L-Glutamate 5-semialdehyde | 0.5 Glutamate(s) 0.5 Proline(s) 1 NADH-redox-potential(m) | 1 L-Glutamate 5-semialdehyde(m) 1 Proton-gradient(m) 1 Na-gradient(c) | - | 4 | - | - | - | - | - | - | 3 | - | 4 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 841 L-Lactate | L-Lactate(s) | PIPES MCES | synthesis of L-Lactate and blood export | 1 Pyruvate(c) 1 NADH-redox-potential(c) | 1 L-Lactate(s) 1 Proton-gradient(c) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |
| 842 L-Octanoylcarnitine | L-Octanoylcarnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic L-Octanoylcarnitine | 2.67 $H_2O$(s) 0.33 Arachidonate(s) 1 L-Carnitine(c) 1 Palmitolate(s) 4 ATP-energy(c) | 0.33 Linoleate(s) 1 L-Octanoylcarnitine(c) 1.67 NADH-redox-potential(c) 4 NADH-redox-potential(p) 1.33 NADPH-redox-potential(r) 0.33 CoA-activated acetyl group(c) 4 CoA-activated acetyl group(p) | 14 | - | 3 | 20 | - | - | - | - | 4 | - | 10 | - |
| 843 L-Oleoylcarnitine | L-Oleoylcarnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic L-Oleoylcarnitine | 1 L-Carnitine(c) 1 Oleate(s) 2 ATP-energy(c) | 1 $H_2O$(s) 1 L-Oleoylcarnitine(c) | 5 | - | - | - | - | - | - | - | 2 | - | - | - |
| 844 L-Palmitoylcarnitine | L-Palmitoylcarnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic L-Palmitoylcarnitine | 1 Palmitate(s) 1 L-Carnitine(c) 2 ATP-energy(c) | 1 $H_2O$(s) 1 L-Palmitoylcarnitine(c) | 5 | - | - | - | - | - | - | - | 2 | - | - | - |
| 845 Lanosterol | Lanosterol(r) | PIPES MCES | synthesis of Golgi/ER Lanosterol | 1 $H_2O$(s) 1 $O_2$(s) 2 Farnesyl-PP(r) 2 NADPH-redox-potential(r) | 4 $P_i$(c) 1 Lanosterol(r) | 1 | - | 5 | - | - | - | - | - | 2 | - | 3 | - |
| 846 Lathosterol | Lathosterol(r) | PIPES MCES | synthesis of Golgi/ER Lathosterol | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 9 NADPH-redox-potential(r) | 5 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Lathosterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 14 | - | - | - | - | - | 3 | - | 5 | - |
| 847 Lauroyl-CoA | Lauroyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Lauroyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Lauroyl-CoA(m) 3 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 Proton-gradient(c) 12 Proton-gradient(m) 5 Na-gradient(c) 2 CoA-activated acetyl group(m) | 46 | 11 | - | - | - | - | - | - | 11 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 848 Linoleate | Linoleate(s) | PIPES MCES | synthesis of Linoleate and blood export | 1.67 $H_2O$(s) 0.33 Phenylalanine(s) 1 Arachidonate(s) 0.67 Farnesyl-PP(r) 3.67 ATP-energy(c) 1 NADPH-redox-potential(c) | 1.33 $P_i$(c) 0.67 $CO_2$(s) 0.33 Tyrosine(s) 0.33 Cholesterol(b) 1 Linoleate(s) 0.33 NADH-redox-potential(r) 2 NADH-redox-potential(c) 0.33 NADPH-redox-potential(r) 0.33 THF-activated methyl group(c) 1 CoA-activated acetyl group(c) | 19 | - | 18 | - | - | - | - | - | 5 | 1 | 9 | - |
| 849 Linoleoyl-CoA | Linoleoyl-CoA(c) | PIPES MCES | synthesis of cytosolic Linoleoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Linoleoyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 11 | - | - | - |
| 850 Malate | Malate(c) | PIPES MCES | synthesis of cytosolic Malate | 1 Pyruvate(c) 1 Pyruvate(m) 1 NADPH-redox-potential(c) | 1 Malate(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 2 | 3 | - | - | - | - | - | - | - | - | 1 | - |
| 851 Malonyl-ACP | Malonyl-ACP(c) | PIPES MCES | synthesis of cytosolic Malonyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 625 ATP-energy(c) 9 Proton-gradient(c) 1 CoA-activated acetyl group(c) | 3 $H_2O$(s) 1 Malonyl-ACP(c) 82 Na-gradient(c) | 17 | - | - | - | - | - | - | - | 23 | - | - | 1 |
| 852 Malonyl-Carnitin | Malonyl-Carnitin(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic Malonyl-Carnitin | 1 Pyruvate(m) 1 L-Carnitine(c) 1 ATP-energy(c) 1 CoA-activated acetyl group(c) | 1 NADH-redox-potential(m) 1 Malonyl-Carnitin(c) 1 CoA-activated acetyl group(m) | 6 | 3 | - | - | - | - | - | - | - | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 853 Malonyl-CoA | Malonyl-CoA(c) | PIPES MCES | synthesis of cytosolic Malonyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) 1 CoA-activated acetyl group(c) | 5.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Malonyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 46 | - | - | - | - | - | - | - | 10 | - | - | - |
| 854 Maltose | Maltose(s) | PIPES MCES | synthesis of Maltose and blood export | 2 Glucose(s) | 1 $H_2O$(s) 1 Maltose(s) | - | - | - | - | - | - | 1 | - | - | - | - | - |
| 855 Mercaptopyruvate | Mercaptopyruvate(c) | PIPES MCES | synthesis of cytosolic Mercaptopyruvate | 1 Pyruvate(c) 1 Cysteine(s) | 1 Alanine(s) 1 Mercaptopyruvate(c) 1 Na-gradient(c) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 856 Methacrylyl-CoA | Methacrylyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Methacrylyl-CoA | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 1 Valine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.2 ATP-energy(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 Methacrylyl-CoA(m) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 1 NADPH-redox-potential(m) 5 Proton-gradient(m) 5 Na-gradient(c) | 43 | 6 | - | - | - | - | - | - | 11 | - | 8 | - |
| 857 Methylmalonyl-CoA | Methylmalonyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Methylmalonyl-CoA | 2.17 $P_i$(c) 1 Pyruvate(m) 1 Glycine(s) 1 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 Methylmalonyl-CoA(m) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 Proton-gradient(c) 4 Na-gradient(c) | 42 | 8 | - | - | - | - | - | - | 10 | - | 3 | - |
| 858 Myristoyl-CoA | Myristoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Myristoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Palmitate(s) 0.5 Cystine(s) 1 Pantothenate(s) 0.5 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Myristoyl-CoA(m) 2.5 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 6 Proton-gradient(m) 3 Na-gradient(c) 1 CoA-activated acetyl group(m) | 47 | 7 | - | - | - | - | - | - | 12 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot | |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 859 N-(omega)-Hydroxyarginine | N-(omega)-Hydroxyarginine(c) | PIPES MCES | synthesis of cytosolic N-(omega)-Hydroxyarginine | 1 $O_2$(s) 1 Arginine(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 N-(omega)-Hydroxyarginine(c) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 860 N-Acetyl-D-mannosamine | N-Acetyl-D-mannosamine(s) | PIPES MCES | synthesis of N-Acetyl-D-mannosamine and blood export | 1 $NH_3$(s) 1 Glucose-6P(c) 2 ATP-energy(c) 1 CoA-activated acetyl group(c) | 1 $P_i$(c) 1 N-Acetyl-D-mannosamine(s) | 10 | - | 2 | - | - | - | - | - | 2 | - | 3 | - |
| 861 N-Acetylglucosamine-1P | N-Acetylglucosamine-1P(c) | PIPES MCES | synthesis of cytosolic N-Acetylglucosamine-1P | 1 Glutamine(s) 1 Glucose-6P(c) 1 CoA-activated acetyl group(c) | 1 Glutamate(s) 1 N-Acetylglucosamine-1P(c) | 5 | - | - | - | - | - | - | - | 2 | - | - | - |
| 862 N-Acetylmannosamine-6P | N-Acetylmannosamine-6P(c) | PIPES MCES | synthesis of cytosolic N-Acetylmannosamine-6P | 1 Glutamine(s) 1 Glucose-6P(c) 2 ATP-energy(c) 1 CoA-activated acetyl group(c) | 1 Glutamate(s) 1 N-Acetylmannosamine-6P(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 863 N-Acetylneuraminate | N-Acetylneuraminate(c) | PIPES MCES | synthesis of cytosolic N-Acetylneuraminate | 1 $NH_3$(s) 1 Pyruvate(c) 1 Glucose-6P(c) 3 ATP-energy(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 1 $P_i$(c) 1 N-Acetylneuraminate(c) 1 NADH-redox-potential(c) | 19 | - | - | - | - | - | - | - | 1 | - | - | - |
| 864 N-Acetylneuraminate-9P | N-Acetylneuraminate-9P(c) | PIPES MCES | synthesis of cytosolic N-Acetylneuraminate-9P | 1 Pyruvate(c) 1 Glutamine(s) 1 Glucose-6P(c) 3 ATP-energy(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 1 Glutamate(s) 1 N-Acetylneuraminate-9P(c) 1 NADH-redox-potential(c) | 18 | - | - | - | - | - | - | - | 2 | - | - | - |
| 865 N-Carbamoyl-L-aspartate | N-Carbamoyl-L-aspartate(c) | PIPES MCES | synthesis of cytosolic N-Carbamoyl-L-aspartate | 1 Pyruvate(m) 1 Asparagine(s) 3 ATP-energy(c) | 1 N-Carbamoyl-L-aspartate(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 7 | 3 | - | - | - | - | - | - | 1 | - | 1 | - |
| 866 N-Formimino-L-glutamate | N-Formimino-L-glutamate(c) | PIPES MCES | synthesis of cytosolic N-Formimino-L-glutamate | 1 $H_2O$(s) 0.5 Glutamate(s) 0.5 Histidine(s) 0.5 THF-activated methyl group(c) | 1 N-Formimino-L-glutamate(c) 0.5 NADH-redox-potential(c) 0.5 NADPH-redox-potential(c) 1 Na-gradient(c) | 10 | - | - | - | - | - | - | - | 4 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 867 N-Formyl-GAR | N-Formyl-GAR(c) | PIPES MCES | synthesis of cytosolic N-Formyl-GAR | 0.17 $P_i$(c) 1 Glycine(s) 1 Glutamine(s) 0.83 Glucose-6P(c) 3.17 ATP-energy(c) 1 Proton-gradient(c) 1 THF-activated methyl group(c) | 0.17 $H_2O$(s) 1 Glutamate(s) 1 N-Formyl-GAR(c) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) | 22 | - | - | - | - | - | - | - | 5 | - | - | - |
| 868 N-Methylethanolamine-P | N-Methylethanolamine-P(c) | PIPES MCES | synthesis of cytosolic N-Methylethanolamine-P | 1 $P_i$(c) 1 Ethanolamine(c) 1 Activated methyl group(c) 1 ATP-energy(c) | 1 $H_2O$(s) 1 N-Methylethanolamine-P(c) | 4 | - | - | - | - | - | - | - | 1 | - | - | - |
| 869 N-Pantothenoylcysteine | N-Pantothenoylcysteine(c) | PIPES MCES | synthesis of cytosolic N-Pantothenoylcysteine | 1 Cysteine(s) 1 Pantothenate(s) 2 ATP-energy(c) | 1 $H_2O$(s) 1 N-Pantothenoylcysteine(c) 1 Na-gradient(c) | 7 | - | - | - | - | - | - | - | 4 | - | - | - |
| 870 NADH | NADH(c) | PIPES MCES | synthesis of cytosolic NADH | 0.33 $P_i$(c) 1 Glycine(s) 1.67 Glucose-6P(c) 2 Asparagine(s) 1 Nicotinamide(s) 16.3 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 3.33 $H_2O$(s) 1 NADH(c) 1 $CO_2$(s) 2 Pyruvate(c) 1 NADH-redox-potential(c) 4 NADPH-redox-potential(c) | 40 | - | - | - | - | - | - | - | 6 | - | - | - |
| 871 NADPH | NADPH(c) | PIPES MCES | synthesis of cytosolic NADPH | 1.33 $P_i$(c) 1 Glycine(s) 1.67 Glucose-6P(c) 2 Asparagine(s) 1 Nicotinamide(s) 17.3 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 4.33 $H_2O$(s) 1 NADPH(c) 1 $CO_2$(s) 2 Pyruvate(c) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 41 | - | - | - | - | - | - | - | 6 | - | - | - |
| 872 NeuNGc | NeuNGc(c) | PIPES MCES | synthesis of cytosolic NeuNGc | 1 $O_2$(s) 1 Pyruvate(c) 1 Glutamine(s) 1 Glucose-6P(c) 3 ATP-energy(c) 1 NADPH-redox-potential(c) 1 CoA-activated acetyl group(c) | 1 $P_i$(c) 1 Glutamate(s) 1 NeuNGc(c) 2 NADH-redox-potential(c) | 20 | - | - | - | - | - | - | - | 3 | - | - | - |
| 873 Nicotinamide D-ribonucleotide | Nicotinamide D-ribonucleotide(c) | PIPES MCES | synthesis of cytosolic Nicotinamide D-ribonucleotide | 0.17 $P_i$(c) 0.83 Glucose-6P(c) 1 Nicotinamide(s) 2.17 ATP-energy(c) | 1.17 $H_2O$(s) 1 Nicotinamide D-ribonucleotide(c) | 14 | - | - | - | - | - | - | - | 2 | - | - | - |
| 874 Nicotinate | Nicotinate(s) | PIPES MCES | synthesis of Nicotinate and blood export | 1 Glutamate(s) 1 Nicotinamide(s) 1 ATP-energy(c) | 1 Glutamine(s) 1 Nicotinate(s) 1 Na-gradient(c) | 5 | - | - | - | - | - | - | - | 5 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 875 Nicotinate D-ribonucleoside | Nicotinate D-ribonucleoside(c) | PIPES MCES | synthesis of cytosolic Nicotinate D-ribonucleoside | 1 Glutamate(s) 0.83 Glucose-6P(c) 1 Nicotinamide(s) 3.17 ATP-energy(c) | 0.17 $H_2O$(s) 0.83 $P_i$(c) 1 Glutamine(s) 1 Nicotinate D-ribonucleoside(c) 1 Na-gradient(c) | 17 | - | - | - | - | - | - | - | 5 | - | - | - |
| 876 Nicotinate(r)ibonucleotide | Nicotinate ribonucleotide(c) | PIPES MCES | synthesis of cytosolic Nicotinate ribonucleotide | 0.17 $P_i$(c) 1 Glutamate(s) 0.83 Glucose-6P(c) 1 Nicotinamide(s) 3.17 ATP-energy(c) | 1.17 $H_2O$(s) 1 Glutamine(s) 1 Nicotinate ribonucleotide(c) 1 Na-gradient(c) | 16 | - | - | - | - | - | - | - | 5 | - | - | - |
| 877 O-Acetylcarnitine | O-Acetylcarnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic O-Acetylcarnitine | 1 L-Carnitine(c) 1 CoA-activated acetyl group(c) | 1 O-Acetylcarnitine(c) | 2 | - | - | - | - | - | - | - | - | - | - | - |
| 878 O-Butanoylcarnitine | O-Butanoylcarnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic O-Butanoylcarnitine | 2.63 $O_2$(s) 0.75 Palmitate(s) 1 L-Carnitine(c) 0.25 Palmitate(s) 2 ATP-energy(c) | 6.25 NADH-redox-potential(m) 0.75 FADH-redox-potential(c) 31.5 Proton-gradient(m) 1 O-Butanoylcarnitine(c) 6.25 CoA-activated acetyl group(m) | 8 | 40 | - | - | - | - | - | - | 3 | - | 12 | - |
| 879 O-Propanoylcarnitine | O-Propanoylcarnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic O-Propanoylcarnitine | 1 Glutamate(s) 1 Threonine(s) 1 L-Carnitine(c) 1 ATP-energy(c) 1 Proton-gradient(m) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Glutamine(s) 1 NADH-redox-potential(m) 1 O-Propanoylcarnitine(c) 2 Na-gradient(c) | 4 | 2 | - | - | - | - | - | - | 6 | - | 5 | - |
| 880 OAA | OAA(c) | PIPES MCES | synthesis of cytosolic OAA | 1 Pyruvate(c) 1 Pyruvate(m) 1 NADPH-redox-potential(c) | 1 OAA(c) 1 NADH-redox-potential(c) 1 NADH-redox-potential(m) 1 CoA-activated acetyl group(m) | 4 | 3 | - | - | - | - | - | - | - | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 881 Octanoyl-ACP | Octanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic Octanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 627 ATP-energy(c) 6 NADPH-redox-potential(c) 3 Proton-gradient(c) 4 CoA-activated acetyl group(c) | 6 $H_2O$(s) 1 $CO_2$(s) 1 Octanoyl-ACP(c) 66 Na-gradient(c) | 31 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 882 Octanoyl-CoA | Octanoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Octanoyl-CoA | 0.5 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Octanoyl-CoA(m) 2 NADH-redox-potential(c) 5 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 6 Proton-gradient(m) 3 Na-gradient(c) 5 CoA-activated acetyl group(m) | 44 | 22 | - | - | - | - | - | - | 12 | - | 7 | - |
| 883 Oleoyl-CoA | Oleoyl-CoA(c) | PIPES MCES | synthesis of cytosolic Oleoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Oleate(s) 1 Pantothenate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Oleoyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 11 | - | - | - |
| 884 Orotate | Orotate(s) | PIPES MCES | synthesis of Orotate and blood export | 0.33 $O_2$(s) 0.5 Pyruvate(m) 1 Aspartate(s) 1 Glutamine(s) 0.33 Proline(s) 2 ATP-energy(c) 0.5 THF-activated methyl group(c) | 1.33 Glutamate(s) 1 Orotate(s) 0.5 NADH-redox-potential(c) 0.83 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 4 Proton-gradient(m) 1.33 Na-gradient(c) 0.5 CoA-activated acetyl group(m) | 13 | 6 | - | - | - | - | - | - | 7 | - | 7 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 885 Orotidine-5P | Orotidine-5P(c) | PIPES MCES | synthesis of cytosolic Orotidine-5P | 0.33 $O_2$(s) 1 Aspartate(s) 1 Glutamine(s) 1 Glucose-6P(c) 0.33 Proline(s) 4 ATP-energy(c) | 1 $H_2O$(s) 1.33 Glutamate(s) 1 Orotidine-5P(c) 0.33 NADH-redox-potential(m) 2 NADPH-redox-potential(c) 1 Proton-gradient(c) 4 Proton-gradient(m) 2.33 Na-gradient(c) | 15 | 4 | - | - | - | - | - | - | 8 | - | 6 | - |
| 886 Oxalosuccinate | Oxalosuccinate(c) | PIPES MCES | synthesis of cytosolic Oxalosuccinate | 1 Pyruvate(c) 1 Pyruvate(m) 1 Glutamate(s) | 1 Alanine(s) 1 Oxalosuccinate(c) 1 NADH-redox-potential(m) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 2 | 3 | - | - | - | - | - | - | 3 | - | 1 | - |
| 887 Oxidized thioredoxin | Oxidized thioredoxin(c) | PIPES MCES | synthesis of cytosolic Oxidized thioredoxin | 10 Glutamate(s) 5 Glycine(s) 8 Alanine(s) 12 Lysine(s) 7 Aspartate(s) 5 Glutamine(s) 7 Serine(s) 3 Methionine(s) 1 Tryptophan(s) 9 Phenylalanine(s) 1 Tyrosine(s) 5 Cysteine(s) 6 Leucine(s) 1 Histidine(s) 3 Proline(s) 3 Asparagine(s) 11 Valine(s) 4 Threonine(s) 4 Isoleucine(s) 525 ATP-energy(c) 6 Proton-gradient(c) | 1 Oxidized thioredoxin(c) 1 NADPH-redox-potential(c) 58 Na-gradient(c) | 5 | - | - | - | - | - | - | - | 21 | - | - | 1 |
| 888 PAP | PAP(c) | PIPES MCES | synthesis of cytosolic PAP | 1.17 $P_i$(c) 1 Glycine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 12.2 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 1 PAP(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 40 | - | - | - | - | - | - | - | 6 | - | - | - |
| 889 PE-PS-VLDL-pool | PE-PS-VLDL-pool(c) | PIPES MCES | synthesis of cytosolic PE-PS-VLDL-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 1 Ethanolamine(c) 0.53 Arachidonate(s) 0.09 Palmitate(s) 0.09 Oleate(s) 1.25 Stearate(s) 0.05 Linoleate(s) 7.5 ATP-energy(c) 1 NADH-redox-potential(c) | 3.5 $H_2O$(s) 1 PE-PS-VLDL-pool(c) | 28 | - | - | - | - | - | - | - | 6 | - | - | - |
| 890 PEP | PEP(c) | PIPES MCES | synthesis of cytosolic PEP | 1 $P_i$(c) 1 Pyruvate(c) 1 ATP-energy(c) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 PEP(c) 1 NADH-redox-potential(c) | 7 | - | - | - | - | - | - | - | 1 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 891 PG-CL-pool | PG-CL-pool(m) | PIPES MCES | synthesis of mitochondrial PG-CL-pool | 1 Glucose-6P(c) 0.09 Palmitate(s) 0.28 Oleate(s) 0.04 Stearate(s) 1.5 Linoleate(s) 0.1 Palmitolate(s) 5 ATP-energy(c) 2 ATP-energy(m) 2 NADH-redox-potential(c) 1 Proton-gradient(m) | 3 $H_2O$(s) 1 PG-CL-pool(m) | 15 | 9 | - | - | - | - | - | - | 6 | - | 5 | - |
| 892 PGP-CL-pool | PGP-CL-pool(m) | PIPES MCES | synthesis of mitochondrial PGP-CL-pool | 1 $P_i$(c) 1 Glucose-6P(c) 0.09 Palmitate(s) 0.28 Oleate(s) 0.04 Stearate(s) 1.5 Linoleate(s) 0.1 Palmitolate(s) 5 ATP-energy(c) 2 ATP-energy(m) 2 NADH-redox-potential(c) 2 Proton-gradient(m) | 4 $H_2O$(s) 1 PGP-CL-pool(m) | 15 | 8 | - | - | - | - | - | - | 6 | - | 6 | - |
| 893 $PP_i$ | $PP_i$(c) | PIPES MCES | synthesis of $PP_i$ | 1.91 $P_i$(c) 0.09 Glucose-6P(c) 1 ATP-energy(c) | 0.91 $H_2O$(s) 1 $PP_i$(c) 0.09 Glucose(s) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 894 PRPP | PRPP(c) | PIPES MCES | synthesis of PRPP | 2.17 $P_i$(c) 0.83 Glucose-6P(c) 2.17 ATP-energy(c) | 2.17 $H_2O$(s) 1 PRPP(c) | 12 | - | - | - | - | - | - | - | 1 | - | - | - |
| 895 Palmitoyl-CoA | Palmitoyl-CoA(c) | PIPES MCES | synthesis of cytosolic Palmitoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Palmitate(s) 0.5 Cystine(s) 1 Pantothenate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Palmitoyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 11 | - | - | - |
| 896 Pantetheine | Pantetheine(c) | PIPES MCES | synthesis of cytosolic Pantetheine | 1 Cysteine(s) 1 Pantothenate(s) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Pantetheine(c) 1 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 5 | - | - | - |
| 897 Phosphatidate-Bile-PC-pool | Phosphatidate-Bile-PC-pool(c) | PIPES MCES | synthesis of cytosolic Phosphatidate-Bile-PC-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.11 Arachidonate(s) 0.83 Palmitate(s) 0.24 Oleate(s) 0.11 Stearate(s) 0.66 Linoleate(s) 0.05 Palmitolate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 Phosphatidate-Bile-PC-pool(c) | 24 | - | - | - | - | - | - | - | 7 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 898 Phosphatidate-CL-pool | Phosphatidate-CL-pool(m) | PIPES MCES | synthesis of mitochondrial Phosphatidate-CL-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.09 Palmitate(s) 0.28 Oleate(s) 0.04 Stearate(s) 1.5 Linoleate(s) 0.1 Palmitolate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) 1 Proton-gradient(m) | 2.5 $H_2O$(s) 1 Phosphatidate-CL-pool(m) | 15 | 2 | - | - | - | - | - | - | 6 | - | 5 | - |
| 899 Phosphatidate-VLDL-PC-pool | Phosphatidate-VLDL-PC-pool(c) | PIPES MCES | synthesis of cytosolic Phosphatidate-VLDL-PC-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.17 Arachidonate(s) 0.7 Palmitate(s) 0.27 Oleate(s) 0.3 Stearate(s) 0.55 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 Phosphatidate-VLDL-PC-pool(c) | 22 | - | - | - | - | - | - | - | 6 | - | - | - |
| 900 Phosphatidate-VLDL-PE-pool | Phosphatidate-VLDL-PE-pool(c) | PIPES MCES | synthesis of cytosolic Phosphatidate-VLDL-PE-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.6 Arachidonate(s) 0.34 Palmitate(s) 0.17 Oleate(s) 0.54 Stearate(s) 0.36 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 Phosphatidate-VLDL-PE-pool(c) | 22 | - | - | - | - | - | - | - | 6 | - | - | - |
| 901 Phosphatidate-VLDL-PI-pool | Phosphatidate-VLDL-PI-pool(c) | PIPES MCES | synthesis of cytosolic Phosphatidate-VLDL-PI-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.51 Arachidonate(s) 0.16 Palmitate(s) 0.32 Oleate(s) 0.85 Stearate(s) 0.16 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 Phosphatidate-VLDL-PI-pool(c) | 22 | - | - | - | - | - | - | - | 6 | - | - | - |
| 902 Phosphatidate-VLDL-PS-pool | Phosphatidate-VLDL-PS-pool(c) | PIPES MCES | synthesis of cytosolic Phosphatidate-VLDL-PS-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.53 Arachidonate(s) 0.09 Palmitate(s) 0.09 Oleate(s) 1.25 Stearate(s) 0.05 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 Phosphatidate-VLDL-PS-pool(c) | 22 | - | - | - | - | - | - | - | 6 | - | - | - |
| 903 Phosphatidate-VLDL-SM-pool | Phosphatidate-VLDL-SM-pool(c) | PIPES MCES | synthesis of cytosolic Phosphatidate-VLDL-SM-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.03 Arachidonate(s) 1.42 Palmitate(s) 0.15 Oleate(s) 0.34 Stearate(s) 0.06 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 Phosphatidate-VLDL-SM-pool(c) | 22 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 904 Phosphatidate-VLDL-TG-pool | Phosphatidate-VLDL-TG-pool(c) | PIPES MCES | synthesis of cytosolic Phosphatidate-VLDL-TG-pool | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.06 Arachidonate(s) 0.83 Palmitate(s) 0.6 Oleate(s) 0.13 Stearate(s) 0.39 Linoleate(s) 4.5 ATP-energy(c) 1 NADH-redox-potential(c) | 2.5 $H_2O$(s) 1 Phosphatidate-VLDL-TG-pool(c) | 22 | - | - | - | - | - | - | - | 6 | - | - | - |
| 905 Phosphocholine | Phosphocholine(c) | PIPES MCES | synthesis of cytosolic Phosphocholine | 1 $P_i$(c) 1 Choline(c) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Phosphocholine(c) | 2 | - | - | - | - | - | - | - | 1 | - | - | - |
| 906 Phosphodimethylethanolamine | Phosphodimethylethanolamine(c) | PIPES MCES | synthesis of cytosolic Phosphodimethylethanolamine | 1 $P_i$(c) 1 Choline(c) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Activated methyl group(c) 1 Phosphodimethylethanolamine(c) | 4 | - | - | - | - | - | - | - | 1 | - | - | - |
| 907 Phosphopantetheine | Phosphopantetheine(c) | PIPES MCES | synthesis of cytosolic Phosphopantetheine | 1 $P_i$(c) 1 Cysteine(s) 1 Pantothenate(s) 1 ATP-energy(c) | 2 $H_2O$(s) 1 $CO_2$(s) 1 Phosphopantetheine(c) 1 Na-gradient(c) | 6 | - | - | - | - | - | - | - | 5 | - | - | - |
| 908 Porphobilinogen | Porphobilinogen(c) | PIPES MCES | synthesis of cytosolic Porphobilinogen | 1 Pyruvate(m) 2 Glutamate(s) 1 Serine(s) 2 Proton-gradient(m) | 2 $H_2O$(s) 2 $CO_2$(s) 1 Aspartate(s) 1 Porphobilinogen(c) 2 NADH-redox-potential(m) 1 Proton-gradient(c) 3 Na-gradient(c) | 1 | 9 | - | - | - | - | - | - | 7 | - | 6 | - |
| 909 Presqualene-PP | Presqualene-PP(r) | PIPES MCES | synthesis of Golgi/ER Presqualene-PP | 1 $H_2O$(s) 2 Farnesyl-PP(r) | 2 $P_i$(c) 1 Presqualene-PP(r) | 1 | - | 1 | - | - | - | - | - | 1 | - | 1 | - |
| 910 Propanoate | Propanoate(s) | PIPES MCES | synthesis of Propanoate and blood export | 1 Aspartate(s) 1 Threonine(s) 1 ATP-energy(c) 1 Proton-gradient(m) | 1 $CO_2$(s) 1 Asparagine(s) 1 Propanoate(s) 1 NADH-redox-potential(m) 1 Proton-gradient(c) 2 Na-gradient(c) | 5 | 2 | - | - | - | - | - | - | 8 | - | 5 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 911 Propanoyl-CoA | Propanoyl-CoA(c) | PIPES MCES | synthesis of cytosolic Propanoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 1.5 Aspartate(s) 0.5 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Asparagine(s) 1 Threonine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.7 ATP-energy(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 Propanoyl-CoA(c) 1 NADH-redox-potential(m) 5.5 NADPH-redox-potential(c) 4.5 Na-gradient(c) | 44 | 2 | - | - | - | - | - | - | 10 | - | 5 | - |
| 912 Protein(l)ysine | Protein lysine(c) | PIPES MCES | synthesis of cytosolic Protein lysine | 1 Lysine(s) | 1 Protein lysine(c) | 1 | - | - | - | - | - | - | - | 1 | - | - | - |
| 913 Protoporphyrin | Protoporphyrin(m) | PIPES MCES | synthesis of mitochondrial Protoporphyrin | 2.5 $O_2$(s) 4 Pyruvate(m) 10.5 Glutamate(s) 4 Serine(s) 1.5 Proline(s) 4 ATP-energy(c) | 14 $H_2O$(s) 14 $CO_2$(s) 4 Aspartate(s) 4 Glutamine(s) 1 Protoporphyrin(m) 4 NADH-redox-potential(c) 4 NADH-redox-potential(m) 2 Proton-gradient(m) 10.5 Na-gradient(c) | 10 | 11 | - | - | - | - | - | - | 8 | - | 10 | - |
| 914 Protoporphyrinogen IX | Protoporphyrinogen IX(c) | PIPES MCES | synthesis of cytosolic Protoporphyrinogen IX | 1 $O_2$(s) 4 Pyruvate(m) 12 Glutamate(s) 4 Serine(s) 4 ATP-energy(c) 4 NADPH-redox-potential(m) 4 Proton-gradient(m) | 14 $H_2O$(s) 14 $CO_2$(s) 4 Aspartate(s) 4 Glutamine(s) 1 Protoporphyrinogen IX(c) 4 NADH-redox-potential(c) 8 NADH-redox-potential(m) 12 Na-gradient(c) | 10 | 8 | - | - | - | - | - | - | 7 | - | 6 | - |
| 915 Provitamin D3 | Provitamin D3(r) | PIPES MCES | synthesis of Golgi/ER Provitamin D3 | 8 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 10 NADPH-redox-potential(r) | 7 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Provitamin D3(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 15 | - | - | - | - | - | 3 | - | 5 | - |
| 916 Pyridoxal | Pyridoxal(s) | PIPES MCES | synthesis of Pyridoxal and blood export | 0.5 $O_2$(s) 1 Pyridoxine(s) | 1 $H_2O$(s) 1 Pyridoxal(s) | 2 | - | - | - | - | - | - | - | 4 | - | - | - |
| 917 Pyridoxine-P | Pyridoxine-P(c) | PIPES MCES | synthesis of cytosolic Pyridoxine-P | 1 $P_i$(c) 1 Pyridoxine(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Pyridoxine-P(c) | 2 | - | - | - | - | - | - | - | 2 | - | - | - |
| 918 Quinolinate | Quinolinate(c) | PIPES MCES | synthesis of cytosolic Quinolinate | 1 Pyruvate(m) 1 Glutamate(s) 1 Nicotinamide(s) 1 ATP-energy(c) | 1 Glutamine(s) 1 Quinolinate(c) 1 NADH-redox-potential(m) 1 Na-gradient(c) 1 CoA-activated acetyl group(m) | 5 | 3 | - | - | - | - | - | - | 4 | - | 1 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 919 Ribose-1P | Ribose-1P(c) | PIPES MCES | synthesis of cytosolic Ribose-1P | 0.17 $P_i$(c) 0.83 Glucose-6P(c) 0.17 ATP-energy(c) | 0.17 $H_2O$(s) 1 Ribose-1P(c) | 11 | - | - | - | - | - | - | - | 1 | - | - | - |
| 920 Ribose-5P | Ribose-5P(c) | PIPES MCES | synthesis of cytosolic Ribose-5P | 0.17 $P_i$(c) 0.83 Glucose-6P(c) 0.17 ATP-energy(c) | 0.17 $H_2O$(s) 1 Ribose-5P(c) | 10 | - | - | - | - | - | - | - | 1 | - | - | - |
| 921 Ribulose-5P | Ribulose-5P(c) | PIPES MCES | synthesis of cytosolic Ribulose-5P | 0.14 $P_i$(c) 0.86 Glucose-6P(c) 0.14 ATP-energy(c) | 0.14 $CO_2$(s) 1 Ribulose-5P(c) 0.29 NADPH-redox-potential(c) | 14 | - | - | - | - | - | - | - | 1 | - | - | - |
| 922 SAH | SAH(c) | PIPES MCES | synthesis of cytosolic SAH | 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 1 Methionine(s) 0.83 Glucose-6P(c) 9.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 0.83 $P_i$(c) 1 $CO_2$(s) 1 SAH(c) 2 Pyruvate(c) 2 Glutamate(s) 1 Activated methyl group(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 3 Na-gradient(c) | 36 | - | - | - | - | - | - | - | 9 | - | - | - |
| 923 SAICAR | SAICAR(c) | PIPES MCES | synthesis of cytosolic SAICAR | 1 Glycine(s) 1 Aspartate(s) 2 Glutamine(s) 1 Glucose-6P(c) 6 ATP-energy(c) 1 THF-activated methyl group(c) | 1 $H_2O$(s) 2 Glutamate(s) 1 SAICAR(c) 1 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Proton-gradient(c) 3 Na-gradient(c) | 21 | - | - | - | - | - | - | - | 7 | - | - | - |
| 924 SAM | SAM(c) | PIPES MCES | synthesis of cytosolic SAM | 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 1 Methionine(s) 0.83 Glucose-6P(c) 9.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 0.83 $P_i$(c) 1 $CO_2$(s) 1 SAM(c) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 3 Na-gradient(c) | 35 | - | - | - | - | - | - | - | 9 | - | - | - |
| 925 Saccharopine | Saccharopine(m) | PIPES MCES | synthesis of mitochondrial Saccharopine | 1 Pyruvate(c) 1 Glutamate(s) 1 Lysine(s) 1 NADPH-redox-potential(m) 1 Proton-gradient(m) | 1 $H_2O$(s) 1 Alanine(s) 1 Saccharopine(m) 1 Na-gradient(c) | 1 | 2 | - | - | - | - | - | - | 4 | - | 5 | - |
| 926 Sarcosine | Sarcosine(s) | PIPES MCES | synthesis of Sarcosine and blood export | 1 Glycine(s) 1 Activated methyl group(c) 1 Proton-gradient(c) | 1 Sarcosine(s) | 2 | - | - | - | - | - | - | - | 3 | - | - | - |
| 927 Sedoheptulose-1,7PP | Sedoheptulose-1,7PP(c) | PIPES MCES | synthesis of cytosolic Sedoheptulose-1,7PP | 0.83 $P_i$(c) 1.17 Glucose-6P(c) 0.83 ATP-energy(c) | 0.83 $H_2O$(s) 1 Sedoheptulose-1,7PP(c) | 10 | - | - | - | - | - | - | - | 1 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 928 Sedoheptulose-7P | Sedoheptulose-7P(c) | PIPES MCES | synthesis of cytosolic Sedoheptulose-7P | 0.17 $H_2O$(s) 1.17 Glucose-6P(c) | 0.17 $P_i$(c) 1 Sedoheptulose-7P(c) 0.17 ATP-energy(c) | 10 | - | - | - | - | - | - | - | 1 | - | - | - |
| 929 Serotonin | Serotonin(s) | PIPES MCES | synthesis of Serotonin and blood export | 1 $O_2$(s) 1 Tryptophan(s) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Serotonin(s) 1 Na-gradient(c) | 4 | - | - | - | - | - | - | - | 6 | - | - | - |
| 930 Sphinganine | Sphinganine(c) | PIPES MCES | synthesis of cytosolic Sphinganine | 1 Serine(s) 1 Palmitate(s) 2 ATP-energy(c) 1 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Sphinganine(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 7 | - | - | - | - | - | - | - | 6 | - | - | - |
| 931 Sphinganine-1P | Sphinganine-1P(c) | PIPES MCES | synthesis of cytosolic Sphinganine-1P | 1 $P_i$(c) 1 Serine(s) 1 Palmitate(s) 3 ATP-energy(c) 1 NADPH-redox-potential(c) | 2 $H_2O$(s) 1 $CO_2$(s) 1 Sphinganine-1P(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 8 | - | - | - | - | - | - | - | 6 | - | - | - |
| 932 Sphingosine | Sphingosine(c) | PIPES MCES | synthesis of cytosolic Sphingosine | 1 Serine(s) 1 Palmitolate(s) 2 ATP-energy(c) 2 NADPH-redox-potential(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Sphingosine(c) 1 NADH-redox-potential(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 13 | - | - | - | - | - | - | - | 6 | - | - | - |
| 933 Sphingosine-1P | Sphingosine-1P(c) | PIPES MCES | synthesis of cytosolic Sphingosine-1P | 1 $P_i$(c) 1 Serine(s) 1 Palmitolate(s) 3 ATP-energy(c) 2 NADPH-redox-potential(c) | 2 $H_2O$(s) 1 $CO_2$(s) 1 Sphingosine-1P(c) 1 NADH-redox-potential(c) 1 Proton-gradient(c) 1 Na-gradient(c) | 14 | - | - | - | - | - | - | - | 6 | - | - | - |
| 934 Squalene | Squalene(r) | PIPES MCES | synthesis of Golgi/ER Squalene | 2 $H_2O$(s) 2 Farnesyl-PP(r) 1 NADPH-redox-potential(r) | 4 $P_i$(c) 1 Squalene(r) | 1 | - | 3 | - | - | - | - | - | 1 | - | 1 | - |
| 935 Squalene 2,3-oxide | Squalene 2,3-oxide(r) | PIPES MCES | synthesis of Golgi/ER Squalene 2,3-oxide | 1 $H_2O$(s) 1 $O_2$(s) 2 Farnesyl-PP(r) 2 NADPH-redox-potential(r) | 4 $P_i$(c) 1 Squalene 2,3-oxide(r) | 1 | - | 4 | - | - | - | - | - | 2 | - | 3 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 936 Stearoyl-ACP | Stearoyl-ACP(c) | PIPES MCES | synthesis of cytosolic Stearoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 632 ATP-energy(c) 16 NADPH-redox-potential(c) 3 Proton-gradient(c) 9 CoA-activated acetyl group(c) | 11 $H_2O$(s) 1 $CO_2$(s) 1 Stearoyl-ACP(c) 66 Na-gradient(c) | 51 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 937 Stearoyl-CoA | Stearoyl-CoA(c) | PIPES MCES | synthesis of cytosolic Stearoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Stearate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 Stearoyl-CoA(c) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 11 | - | - | - |
| 938 Succinate | Succinate(c) | PIPES MCES | synthesis of Succinate and blood export | 1 $H_2O$(s) 1 Pyruvate(c) 1 Glutamate(s) | 1 $CO_2$(s) 1 Alanine(s) 1 Succinate(c) 1 ATP-energy(m) 1 NADH-redox-potential(m) 1 Na-gradient(c) | 1 | 5 | - | - | - | - | - | - | 5 | - | 3 | - |
| 939 Succinyl-CoA | Succinyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Succinyl-CoA | 2.17 $P_i$(c) 1 Pyruvate(m) 1 Glycine(s) 1 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 11.2 ATP-energy(c) 1 NADPH-redox-potential(m) 1 Proton-gradient(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 1 Glutamate(s) 1 Succinyl-CoA(m) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 Na-gradient(c) | 42 | 6 | - | - | - | - | - | - | 10 | - | 3 | - |
| 940 Sulfite degr | -1 Sulfite(c) | PIPES MCES +Sulfate(c) | synthesis of cytosolic Sulfite | 0.5 $O_2$(s) 1 Sulfite(c) | 1 Sulfate(c) 2 Proton-gradient(m) | - | - | - | - | - | - | - | - | 1 | - | 5 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 941 THF-hexaglutamate | THF-hexaglutamate(c) | PIPES MCES | synthesis of cytosolic THF-hexaglutamate | 6 Glutamate(s) 1 Folate(s) 6 ATP-energy(c) 1 NADH-redox-potential(c) 1 NADPH-redox-potential(c) | 1 THF-hexaglutamate(c) 6 Na-gradient(c) | 6 | - | - | - | - | - | - | - | 3 | - | - | - |
| 942 Tetradecanoyl-ACP | Tetradecanoyl-ACP(c) | PIPES MCES | synthesis of cytosolic Tetradecanoyl-ACP | 1 $P_i$(c) 5 Glutamate(s) 6 Glycine(s) 11 Alanine(s) 4 Lysine(s) 8 Aspartate(s) 9 Arginine(s) 7 Glutamine(s) 8 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 3 Cysteine(s) 20 Leucine(s) 1 Histidine(s) 9 Proline(s) 1 Asparagine(s) 11 Valine(s) 6 Threonine(s) 4 Isoleucine(s) 1 Pantothenate(s) 630 ATP-energy(c) 12 NADPH-redox-potential(c) 3 Proton-gradient(c) 7 CoA-activated acetyl group(c) | 9 $H_2O$(s) 1 $CO_2$(s) 1 Tetradecanoyl-ACP(c) 66 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 24 | - | - | 1 |
| 943 Thymidine | Thymidine(s) | PIPES MCES | synthesis of Thymidine and blood export | 0.33 $O_2$(s) 1 Aspartate(s) 0.5 Glucose-6P(c) 0.33 Proline(s) 1 Ethanolamine(c) 6.5 ATP-energy(c) 1 THF-activated methyl group(c) | 2.5 $H_2O$(s) 0.5 $P_i$(c) 0.33 Glutamate(s) 1 Thymidine(s) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 30 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 944 Thymine | Thymine(s) | PIPES MCES | synthesis of Thymine and blood export | 0.33 $O_2$(s) 1 Aspartate(s) 1 Glutamine(s) 0.33 Proline(s) 4 ATP-energy(c) 1 NADH-redox-potential(c) 1 THF-activated methyl group(c) | 1 $H_2O$(s) 1.33 Glutamate(s) 1 Thymine(s) 0.33 NADH-redox-potential(m) 1 NADPH-redox-potential(c) 1 Proton-gradient(c) 4 Proton-gradient(m) 2.33 Na-gradient(c) | 24 | 4 | - | - | - | - | - | - | 9 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 945 Tiglyl-CoA | Tiglyl-CoA(m) | PIPES MCES | synthesis of mitochondrial Tiglyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 1.25 Aspartate(s) 0.25 Glutamine(s) 0.83 Glucose-6P(c) 0.25 Proline(s) 0.75 Asparagine(s) 0.75 Threonine(s) 0.25 Isoleucine(s) 0.5 Cystine(s) 1 Pantothenate(s) 12.9 ATP-energy(c) 1 Proton-gradient(m) 2 THF-activated methyl group(c) 0.75 CoA-activated acetyl group(m) | 6.17 $H_2O$(s) 3 $CO_2$(s) 2 Pyruvate(c) 0.5 Glutamate(s) 1 Tiglyl-CoA(m) 2 NADH-redox-potential(c) 0.75 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 4.25 Na-gradient(c) | 45 | 13 | - | - | - | - | - | - | 12 | - | 7 | - |
| 946 Trehalose | Trehalose(s) | PIPES MCES | synthesis of Trehalose and blood export | 2 Glucose(s) | 1 $H_2O$(s) 1 Trehalose(s) | - | - | - | - | - | - | 1 | - | - | - | - | - |
| 947 Triphosphate degr | -1 Triphosphate(c) | PIPES MCES | degradation of cytosolic Triphosphate | 2 $H_2O$(s) 1 Triphosphate(c) | 3 $P_i$(c) | 2 | - | - | - | - | - | - | - | 1 | - | - | - |
| 948 UDP-N-acetylglucosamine | UDP-N-acetylglucosamine(c) | PIPES MCES | synthesis of cytosolic UDP-N-acetylglucosamine | 0.33 $O_2$(s) 0.17 $P_i$(c) 1 Glutamine(s) 1.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 6.17 ATP-energy(c) 1 CoA-activated acetyl group(c) | 3.17 $H_2O$(s) 1.33 Glutamate(s) 1 UDP-N-acetylglucosamine(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 28 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 949 UDP-activated-N-acetyl-D-galactosamine | UDP-activated-N-acetyl-D-galactosamine(c) | PIPES MCES | synthesis of cytosolic UDP-activated-N-acetyl-D-galactosamine | 1 Glutamine(s) 1 Glucose-6P(c) 1 ATP-energy(c) 1 CoA-activated acetyl group(c) | 1 $P_i$(c) 1 Glutamate(s) 1 UDP-activated-N-acetyl-D-galactosamine(c) | 11 | - | - | - | - | - | - | - | 2 | - | - | - |
| 950 UDP-activated-xylose | UDP-activated-xylose(c) | PIPES MCES | synthesis of cytosolic UDP-activated-xylose | 1 $H_2O$(s) 1 Glucose-6P(c) 1 ATP-energy(c) | 1 $P_i$(c) 1 $CO_2$(s) 2 NADH-redox-potential(c) 1 UDP-activated-xylose(c) | 8 | - | 1 | - | - | - | - | - | 2 | - | 3 | - |
| 951 UMP | UMP(s) | PIPES MCES | synthesis of UMP and blood export | 0.33 $O_2$(s) 2.17 $P_i$(c) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 7.17 ATP-energy(c) | 2.17 $H_2O$(s) 2 $P_i$(s) 0.33 Glutamate(s) 1 UMP(s) 0.33 NADH-redox-potential(m) 1 Proton-gradient(c) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 24 | 4 | - | - | - | - | 2 | - | 8 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 952 Urate | Urate(s) | PIPES MCES | synthesis of Urate and blood export | 1 $NH_3$(s) 1 Aspartate(s) 1 Glutamine(s) 1 Serine(s) 8 ATP-energy(c) 1 THF-activated methyl group(c) | 1 Pyruvate(c) 1 Glutamate(s) 1 Urate(s) 3 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 29 | - | - | - | - | - | - | - | 8 | - | - | - |
| 953 Urocanate | Urocanate(c) | PIPES MCES | synthesis of cytosolic Urocanate | 1 Glutamate(s) 1 Histidine(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 Glutamine(s) 1 Urocanate(c) 2 Na-gradient(c) | 3 | - | - | - | - | - | - | - | 5 | - | - | - |
| 954 UroporphyrinogenIII | Uroporphyrinogen[illegible] | PIPES MCES | synthesis of cytosolic Uroporphyrinogen[illegible] | 4 Pyruvate(m) 12 Glutamate(s) 4 Serine(s) 4 ATP-energy(c) 4 NADPH-redox-potential(m) 4 Proton-gradient(m) | 12 $H_2O$(s) 8 $CO_2$(s) 4 Aspartate(s) 4 Glutamine(s) 1 UroporphyrinogenIII(c) 4 NADH-redox-potential(c) 8 NADH-redox-potential(m) 12 Na-gradient(c) | 8 | 8 | - | - | - | - | - | - | 6 | - | 6 | - |
| 955 Xanthosine | Xanthosine(c) | PIPES MCES | synthesis of cytosolic Xanthosine | 0.83 $NH_3$(s) 1 Glycine(s) 0.17 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 8 ATP-energy(c) 2 THF-activated methyl group(c) | 0.83 $P_i$(c) 1 Pyruvate(c) 0.17 Glutamate(s) 1 Xanthosine(c) 3 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1.17 Proton-gradient(c) 1.17 Na-gradient(c) | 35 | - | - | - | - | - | - | - | 7 | - | - | - |
| 956 Xanthurenate | Xanthurenate(s) | PIPES MCES | synthesis of Xanthurenate and blood export | 2 $O_2$(s) 1 Pyruvate(c) 1 Tryptophan(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 $CO_2$(s) 1 Alanine(s) 1 Xanthurenate(s) 1 Na-gradient(c) | 9 | - | - | - | - | - | - | - | 7 | - | - | - |
| 957 Zymosterol | Zymosterol(r) | PIPES MCES | synthesis of Golgi/ER Zymosterol | 7 $O_2$(s) 2 Farnesyl-PP(r) 1 ATP-energy(c) 8 NADPH-redox-potential(r) | 5 $H_2O$(s) 4 $P_i$(c) 3 $CO_2$(s) 1 Zymosterol(r) 1 NADH-redox-potential(r) 1 NADPH-redox-potential(c) | 5 | - | 12 | - | - | - | - | - | 3 | - | 5 | - |
| 958 cAMP | cAMP(c) | PIPES MCES | synthesis of cytosolic cAMP | 0.17 $P_i$(c) 1 Glycine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 11.2 ATP-energy(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 1 cAMP(c) 2 NADH-redox-potential(c) 4 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 37 | - | - | - | - | - | - | - | 6 | - | - | - |
| 959 cGMP | cGMP(c) | PIPES MCES | synthesis of cytosolic cGMP | 0.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 10.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 cGMP(c) 3 NADH-redox-potential(c) 3 NADPH-redox-potential(c) | 37 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 960 cis-(3S)-hydroxytetradec-7-enoyl-CoA | cis-(3S)-hydroxytetradec-7-enoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial cis-(3S)-hydroxytetradec-7-enoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 FADH-redox-potential(c) 1 cis-(3S)-hydroxytetradec-7-enoyl-CoA(m) 3 Na-gradient(c) 1 CoA-activated acetyl group(m) | 44 | 8 | - | - | - | - | - | - | 11 | - | 3 | - |
| 961 cis-Aconitate | cis-Aconitate(c) | PIPES MCES | synthesis of cytosolic cis-Aconitate | 1 Pyruvate(c) 1 Pyruvate(m) 1 NADPH-redox-potential(c) | 1 cis-Aconitate(c) 2 NADH-redox-potential(m) | 2 | 5 | - | - | - | - | - | - | - | - | 2 | - |
| 962 cis-laur-5-enoyl-CoA | cis-laur-5-enoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial cis-laur-5-enoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 FADH-redox-potential(c) 1 cis-laur-5-enoyl-CoA(m) 3 Na-gradient(c) 2 CoA-activated acetyl group(m) | 44 | 10 | - | - | - | - | - | - | 11 | - | 3 | - |
| 963 cis-myrist-7-enoyl-CoA | cis-myrist-7-enoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial cis-myrist-7-enoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 1 FADH-redox-potential(c) 1 cis-myrist-7-enoyl-CoA(m) 3 Na-gradient(c) 1 CoA-activated acetyl group(m) | 44 | 6 | - | - | - | - | - | - | 11 | - | 3 | - |
| 964 dADP | dADP(c) | PIPES MCES | synthesis of cytosolic dADP | 1.17 $P_i$(c) 1 Glycine(s) 0.83 Glucose-6P(c) 2 Asparagine(s) 10.2 ATP-energy(c) 2 THF-activated methyl group(c) | 3.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 1 dADP(c) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 1 Proton-gradient(c) 2 Na-gradient(c) | 38 | - | - | - | - | - | - | - | 6 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 965 dAMP | dAMP(c) | PIPES MCES | synthesis of cytosolic dAMP | 0.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 7.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 dAMP(c) 2 NADH-redox-potential(c) 3 NADPH-redox-potential(c) 2 Na-gradient(c) | 37 | - | - | - | - | - | - | - | 8 | - | - | - |
| 966 dCDP | dCDP(c) | PIPES MCES | synthesis of cytosolic dCDP | 0.33 $O_2$(s) 1.17 $P_i$(c) 1 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 6.17 ATP-energy(c) 1 NADPH-redox-potential(c) | 4.17 $H_2O$(s) 1.33 Glutamate(s) 1 dCDP(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 28 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 967 dCMP | dCMP(c) | PIPES MCES | synthesis of cytosolic dCMP | 0.33 $O_2$(s) 0.17 $P_i$(c) 1 Glutamine(s) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 6.17 ATP-energy(c) 1 NADPH-redox-potential(c) | 3.17 $H_2O$(s) 1.33 Glutamate(s) 1 dCMP(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 0.33 Na-gradient(c) | 29 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 968 dGDP | dGDP(c) | PIPES MCES | synthesis of cytosolic dGDP | 1.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 9.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 2.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 dGDP(c) 3 NADH-redox-potential(c) 2 NADPH-redox-potential(c) | 37 | - | - | - | - | - | - | - | 6 | - | - | - |
| 969 dGMP | dGMP(c) | PIPES MCES | synthesis of dGMP | 0.17 $P_i$(c) 1 Glycine(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 1 Asparagine(s) 8.17 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 1.17 $H_2O$(s) 1 Pyruvate(c) 2 Glutamate(s) 1 dGMP(c) 3 NADH-redox-potential(c) 2 NADPH-redox-potential(c) | 38 | - | - | - | - | - | - | - | 6 | - | - | - |
| 970 dTDP | dTDP(c) | PIPES MCES | synthesis of dTDP | 0.33 $O_2$(s) 1.5 $P_i$(c) 1 Aspartate(s) 0.5 Glucose-6P(c) 0.33 Proline(s) 1 Ethanolamine(c) 7.5 ATP-energy(c) 1 THF-activated methyl group(c) | 4.5 $H_2O$(s) 0.33 Glutamate(s) 1 dTDP(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 30 | 4 | - | - | - | - | - | - | 6 | - | 6 | - |
| 971 dTMP | dTMP(c) | PIPES MCES | synthesis of dTMP | 0.33 $O_2$(s) 0.5 $P_i$(c) 1 Aspartate(s) 0.5 Glucose-6P(c) 0.33 Proline(s) 1 Ethanolamine(c) 6.5 ATP-energy(c) 1 NADPH-redox-potential(c) 1 THF-activated methyl group(c) | 3.5 $H_2O$(s) 0.33 Glutamate(s) 1 dTMP(c) 1 NADH-redox-potential(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 31 | 4 | - | - | - | - | - | - | 6 | - | 6 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 972 dUDP | dUDP(c) | PIPES MCES | synthesis of cytosolic dUDP | 0.33 $O_2$(s) 1.17 $P_i$(c) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 6.17 ATP-energy(c) 1 NADPH-redox-potential(c) | 4.17 $H_2O$(s) 0.33 Glutamate(s) 1 dUDP(c) 0.33 NADH-redox-potential(m) 1 Proton-gradient(c) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 26 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 973 dUMP | dUMP(c) | PIPES MCES | synthesis of cytosolic dUMP | 0.33 $O_2$(s) 0.5 $P_i$(c) 1 Aspartate(s) 0.5 Glucose-6P(c) 0.33 Proline(s) 1 Ethanolamine(c) 6.5 ATP-energy(c) | 3.5 $H_2O$(s) 0.33 Glutamate(s) 1 dUMP(c) 0.33 NADH-redox-potential(m) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 25 | 4 | - | - | - | - | - | - | 6 | - | 6 | - |
| 974 dUTP | dUTP(c) | PIPES MCES | synthesis of cytosolic dUTP | 0.33 $O_2$(s) 2.17 $P_i$(c) 0.83 Glucose-6P(c) 0.33 Proline(s) 1 Asparagine(s) 7.17 ATP-energy(c) 1 NADPH-redox-potential(c) | 5.17 $H_2O$(s) 0.33 Glutamate(s) 1 dUTP(c) 0.33 NADH-redox-potential(m) 1 Proton-gradient(c) 4 Proton-gradient(m) 1.33 Na-gradient(c) | 27 | 4 | - | - | - | - | - | - | 7 | - | 6 | - |
| 975 gamma-Glutamyl-cysteine | gamma-Glutamyl-cysteine(c) | PIPES MCES | synthesis of cytosolic gamma-Glutamyl-cysteine | 1 Glutamate(s) 1 Cysteine(s) 1 ATP-energy(c) | 1 $H_2O$(s) 1 gamma-Glutamyl-cysteine(c) 1 Na-gradient(c) | 2 | - | - | - | - | - | - | - | 4 | - | - | - |
| 976 gamma-Linolenoyl-CoA | gamma-Linolenoyl-CoA(c) | PIPES MCES | synthesis of cytosolic gamma-Linolenoyl-CoA | 1 $O_2$(s) 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Linoleate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 7.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 1 gamma-Linolenoyl-CoA(c) 1 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 3 Na-gradient(c) | 44 | - | - | - | - | - | - | - | 12 | - | - | - |
| 977 linoleic-Carnitine | linoleic-Carnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic linoleic-Carnitine | 1 L-Carnitine(c) 1 Linoleate(s) 2 ATP-energy(c) | 1 $H_2O$(s) 1 linoleic-Carnitine(c) | 5 | - | - | - | - | - | - | - | 2 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 978 mitoACP | mitoACP(m) | PIPES MCES | synthesis of mitochondrial mitoACP | 1 $P_i$(c) 16.8 Pyruvate(m) 3 Alanine(s) 7 Lysine(s) 2.75 Aspartate(s) 1 Arginine(s) 12 Glutamine(s) 4.5 Serine(s) 5 Methionine(s) 3 Phenylalanine(s) 4 Tyrosine(s) 2 Cysteine(s) 10 Leucine(s) 1 Histidine(s) 5.75 Proline(s) 2 Asparagine(s) 6 Valine(s) 1 Threonine(s) 8 Isoleucine(s) 1 Pantothenate(s) 435.3 ATP-energy(m) 3.75 NADH-redox-potential(c) 17 NADPH-redox-potential(m) 1 Proton-gradient(c) 23.5 Proton-gradient(m) | 21.2 NADH-redox-potential(m) 1 mitoACP(m) 24.8 Na-gradient(c) 8.25 CoA-activated acetyl group(m) | 8 | 24 | - | - | - | - | - | - | 20 | - | 23 | 1 |
| 979 mitoOxidizedThioredoxin | mitoOxidizedThioredoxin(m) | PIPES MCES | synthesis of mitochondrial mitoOxidizedThioredoxin | 6 Glutamate(s) 10 Glycine(s) 11 Alanine(s) 11 Lysine(s) 12 Aspartate(s) 9 Arginine(s) 10 Glutamine(s) 8 Serine(s) 4 Methionine(s) 2 Tryptophan(s) 6 Phenylalanine(s) 2 Tyrosine(s) 3 Cysteine(s) 15 Leucine(s) 3 Histidine(s) 12 Proline(s) 4 Asparagine(s) 17 Valine(s) 12 Threonine(s) 9 Isoleucine(s) 830 ATP-energy(c) 2 Proton-gradient(c) | 1 NADPH-redox-potential(m) 1 mitoOxidizedThioredoxin(m) 102 Na-gradient(c) | 3 | 2 | - | - | - | - | - | - | 22 | - | 1 | 1 |
| 980 palmitoleoyl-Carnitine | palmitoleoyl-Carnitine(c) | PIPES MCES −L-Carnitine(c) | synthesis of cytosolic palmitoleoyl-Carnitine | 1 L-Carnitine(c) 1 Palmitolate(s) 2 ATP-energy(c) | 1 $H_2O$(s) 1 palmitoleoyl-Carnitine(c) | 5 | - | - | - | - | - | - | - | 2 | - | - | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 981 palmitoleoyl-CoA | palmitoleoyl-CoA(c) | PIPES MCES | synthesis of cytosolic palmitoleoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 palmitoleoyl-CoA(c) 3 Na-gradient(c) | 43 | - | - | - | - | - | - | - | 11 | - | - | - |
| 982 sn-Glycerol-3P | sn-Glycerol-3P(c) | PIPES MCES | synthesis of cytosolic sn-Glycerol-3P | 0.5 $P_i$(c) 0.5 Glucose-6P(c) 0.5 ATP-energy(c) 1 NADH-redox-potential(c) | 0.5 $H_2O$(s) 1 sn-Glycerol-3P(c) | 7 | - | - | - | - | - | - | - | 1 | - | - | - |
| 983 trans,cis-dodeca-2,5-dienoyl-CoA | trans,cis-dodeca-2,5-dienoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial trans,cis-dodeca-2,5-dienoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 4.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 2 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 3 FADH-redox-potential(c) 1 trans,cis-dodeca-2,5-dienoyl-CoA(m) 3 Na-gradient(c) 2 CoA-activated acetyl group(m) | 44 | 11 | - | - | - | - | - | - | 11 | - | 3 | - |
| 984 trans,cis-hexadeca-2,9-dienoyl-CoA | trans,cis-hexadeca-2,9-dienoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial trans,cis-hexadeca-2,9-dienoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 FADH-redox-potential(c) 1 trans,cis-hexadeca-2,9-dienoyl-CoA(m) 3 Na-gradient(c) | 44 | 1 | - | - | - | - | - | - | 11 | - | 2 | - |
| 985 trans,cis-myristo-2,7-dienoyl-CoA | trans,cis-myristo-2,7-dienoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial trans,cis-myristo-2,7-dienoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Pantothenate(s) 1 Palmitolate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 5.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 1 NADH-redox-potential(m) 3.5 NADPH-redox-potential(c) 2 FADH-redox-potential(c) 1 trans,cis-myristo-2,7-dienoyl-CoA(m) 3 Na-gradient(c) 1 CoA-activated acetyl group(m) | 44 | 7 | - | - | - | - | - | - | 11 | - | 3 | - |

Continued on next page

C5. Comprehensive list – continued.

| Simulation | Definition | | | Solution | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | exchanges | | reactions | | | | | | | | transport | | Prot |
| | Objective | Contraints | Comment | imports | exports | c | m | r | p | l | n | s | b | s-c | b-c | intra | syn |
| 986 trans,cis-octadeca-2,9-dienoyl-CoA | trans,cis-octadeca-2,9-dienoyl-CoA(m) | PIPES MCES | synthesis of mitochondrial trans,cis-octadeca-2,9-dienoyl-CoA | 2.17 $P_i$(c) 1 Glycine(s) 2 Aspartate(s) 2 Glutamine(s) 0.83 Glucose-6P(c) 0.5 Cystine(s) 1 Oleate(s) 1 Pantothenate(s) 13.2 ATP-energy(c) 1 Proton-gradient(c) 2 THF-activated methyl group(c) | 6.17 $H_2O$(s) 2 $CO_2$(s) 2 Pyruvate(c) 2 Glutamate(s) 2 NADH-redox-potential(c) 3.5 NADPH-redox-potential(c) 1 FADH-redox-potential(c) 1 trans,cis-octadeca-2,9-dienoyl-CoA(m) 3 Na-gradient(c) | 44 | 1 | - | - | - | - | - | - | 11 | - | 2 | - |
| 987 trans-4-Hydroxy-L-proline | trans-4-Hydroxy-L-proline(c) | PIPES MCES −L-1-Pyrroline-3-hydroxy-5-carboxylate(c) | synthesis of cytosolic trans-4-Hydroxy-L-proline | 1 L-1-Pyrroline-3-hydroxy-5-carboxylate(c) 1 NADH-redox-potential(c) | 1 trans-4-Hydroxy-L-proline(c) | 2 | - | - | - | - | - | - | - | - | - | - | - |