Biochemical reactions

Reactions indexed with an asterisk (*) are omitted in the applied metabolic networks.

Glycolysis and citric acid cycle

(1) 1 GLUC + 1 ATP → 1 GLUC6P + 1 ADP + 1 H
(2) 1 GLUC6P → 1 FRUC6P
(3) 0.5 FRUC6P + 0.5 ATP → 1 GAP + 0.5 ADP + 0.5 H
(4) 1 GAP + 0.5 H_2O → 0.5 FRUC6P + 0.5 Pi
(5) 1 GAP + 1 NADH + 1 H_2O + 1 H → 1 GOH + 1 NAD + 1 Pi
(6) 1 GAP + 1 NAD + 1 Pi + 1 ADP → 1 G3P + 1 ATP + 1 NADH + 1 H
(7) 1 G3P → 1 PEP + 1 H_2O
(8) 1 PEP + 1 ADP + 1 H → 1 PYR + 1 ATP
(9)* 1 PYR + 2 ATP + 1 H_2O → 1 PEP + 2 ADP + 1 Pi + 2 H
(10) 1 PYR + 1 NAD + 1 COA → 1 ACCOA + 1 NADH + 1 CO_2
(11) 1 PYR + 1 H → 1 ACET + 1 CO_2
(12) 1 PYR + 1 ATP + 1 H_2O + 1 CO_2 → 1 OAC + 1 ADP + 1 Pi + 2 H
(13) 1 ACET + 1 NAD + 1 H_2O → 1 AC + 1 NADH + 2 H
(14) 1 ACET + 1 NADP + 1 H_2O → 1 AC + 1 NADPH + 2 H
(15) 1 OAC + 1 ACCOA + 1 H_2O → 1 ISOCIT + 1 COA + 1 H
(16) 1 OAC + 1 ATP → 1 PEP + 1 CO_2 + 1 ADP
(17) 1 ISOCIT + 1 NAD → 1 AKG + 1 NADH + 1 CO_2
(18) 1 ISOCIT + 1 NADP → 1 AKG + 1 NADPH + 1 CO_2
(19) 1 AKG + 1 COA + 1 NAD + 1 H → 1 SUCCOA + 1 NADH + 1 CO_2 + 1 H
(20) 1 SUCCOA + 1 ADP + 1 Pi → 1 SUC + 1 ATP + 1 COA
(21) 1 SUC + 1 FAD → 1 FUM + 1 $FADH_2$
(22) 1 FUM + 1 H_2O → 1 MAL
(23) 1 MAL + 1 NAD → 1 OAC + 1 NADH + 1 H
(24) 1 FADH2 + 1 NAD → 1 NADH + 1 H + 1 FAD

PEP phosphotransferase

(25) 1 GLUC(E) + 1 PEP → 1 GLUC6P + 1 PYR

Pentose phosphate pathway

(26) 1 GLUC6P + 2 NADP + 1 H_2O → 1 RIBU5P + 2 NADPH + 1 CO_2 + 2 H
(27) 1 RIBU5P → 1 RIB5P
(28) 1 RIBU5P → 1 XYL5P
(29) 1 RIB5P + 1 XYL5P → 1 SED5P + 1 GAP
(30) 1 SED5P + 1 GAP → 1 FRUC6P + 1 E4P
(31) 1 XYL5P + 1 E4P → 1 FRUC6P + 1 GAP

Glyoxylate shunt

(32) 1 ISOCIT → 1 GLYO + 1 SUC
(33) 1 GLYO + 1 ACCOA + 1 H_2O → 1 MAL + 1 COA + 1 H

Oxidative phosphorylation

(34) 1 NADH + 0.5 O_2 + δ_1ADP + δ_1 Pi + (1 + δ_1) H → (1 + δ_1) H_2O + 1 NAD + δ_1 ATP
(35) 1 NADH + 0.5 O_2 + 1 H → 1 H_2O + 1 NAD
(36) 1 $FADH_2$ + 0.5 O_2 + δ_2 ADP + δ_2 Pi + δ_2 H → (1 + δ_2) H_2O + 1 FAD + δ_2 ATP
(37)* 1 $FADH_2$ + 0.5 O_2 + 3/5 δ_1 ADP + 3/5 δ_1 Pi + 3/5 δ_1 H → (1 + 3/5 δ_1) H_2O + 1 FAD + 3/5 δ_1 ATP
(38)* 1 NADPH + 0.5 O_2 + δ_1 ADP + δ_1 Pi + (1 + δ_1) H → (1 + δ_1) H_2O + 1 NADP + δ_1 ATP

Carbon substrates other than glucose

(39) 1 CIT → 1 ISOCIT
(40) 1 LAC + 1 FAD → 1 PYR + 1 $FADH_2$
(41) 1 GOH + 1 ATP + 1 FAD → 1 GAP + 1 FADH2 + 1 ADP + 1 H
(42) 1 GLUCON + 1 ATP → 1 PYR + 1 GAP + 1 ADP + 1 H_2O + 1 H
(43) 1 ETOH + 1 NAD → 1 ACET + 1 NADH + 1 H
(44) 1 AC + 1 COA + 2 ATP + 1 H_2O → 1 ACCOA + 2 ADP + 2 Pi + 1 H

Transfer of 1-carbon compounds

(45) 1 THF + 1 ATP + 1 NADH + 1 CO_2 → 1 FTHF + 1 ADP + 1 Pi + 1 NAD
(46) 1 THF + 1 CO_2 + 3 NADH + 3 H → 1 MYTHF + 3 NAD + 2 H_2O
(47) 1 THF + 1 CO_2 + 2 NADH + 2 H → 1 MYTHF + 2 NAD + 2 H_2O

Transport

(48) 1 Pi(E) + 2 H(E) → 1 Pi + 2 H
(49) 1 NH_4(E) + 1 H(E) → 1 NH_4 + 1 H
(50) 1 GLUC(E) + 1 H(E) → 1 GLUC + 1 H
(51) 1 SO_4(E) + 3 H(E) → 1 SO4 + 3 H
(52) 1 AC(E) + 1 H(E) → 1 AC + 1 H
(53) 1 LAC(E) + 1 H(E) → 1 LAC + 1 H
(54) 1 PYR(E) + 1 H(E) → 1 PYR + 1 H
(55) 1 GLUCON(E) + 1 H(E) → 1 GLUCON + 1 H
(56) 1 SUC(E) + 2 H(E) → 1 SUC + 2 H
(57) 1 CIT(E) + 3 H(E) → 1 CIT + 3 H

H^+ ATPase

(58) 1 ATP + 1 H_2O → 1 ADP + 1 H(E) + 1 Pi

Amino acid synthesis

(59) 1 AKG + 1 NH_4 + 1 NADPH + 1 H → 1 GLUT + 1 NADP + 1 H_2O
(60) 1 GLUT + 1 NH_4 + 1 ATP → 1 GLUM + 1 ADP + 1 Pi + 1 H
(61) 1 GLUT + 1 ATP + 2 NADPH + 2H → 1 PRO + 1 ADP + 1 Pi + 1 H_2O + 2 NADP
(62) 1 ATP + 1 NH_4 + 1 CO_2 → 1 CARP + 1 ADP + 2 H
(63) 2 GLUT + 1 ACCOA + 4 ATP + 1 NADPH + 1 CARP + 1 ASP + 3 H_2O → 1 ARG + 1 COA + 1 AKG + 1 AC + 4 ADP + 1 FUM + 5 Pi + 1 NADP + 4 H
(64) 2 GLUT + 1 ACCOA + 3 ATP + 2 NADPH + 2 NAD + 3 H_2O → 1 LYS + 1 COA + 1 AKG + 1 CO_2 + 3 ADP + 3 Pi + 2 NADP + 2 H + 2 NADH
(65) 1 ASP + 1 PYR + 2 NADPH + 1 SUCCOA + 1 GLUT + 1 ATP + 2 H → 1 LYS + 1 SUCC + 1 AKG + 1 CO_2 + 2 NADP + 1 COA + 1 ADP + 1 Pi
(66) 1 G3P + 1 GLUT + 1 NAD + 1 H_2O → 1 SER + 1 AKG + 1 Pi + 1 H + 1 NADH
(67) 1 SER + 1 THF → 1 GLY + 1 METHF + 1 H_2O
(68) 1 SER + 1 ACCOA + 1 SO_4 + 4 NADPH + 4 H + 1 ATP → 1 CYS + 1 AC + 1 COA + 4 NADP + 1 ADP + 3 H_2O + 1 Pi

(69) 1 OAC + 1 GLUT → 1 ASP + 1 AKG

(70) 1 ASP + 1 NH_4 + 2 ATP + 1 H_2O → 1 ASN + 2 H + 2 ADP + 2 Pi

(71) 1 ASP + 1 ATP + 2 NADPH + 2 H → 1 HOM + 1 ADP + 1 Pi + 2 NADP

(72) 1 HOM + 1 ATP + 1 H_2O → 1 THR + 1 ADP + 1 Pi + 1 H

(73) 1 HOM + 1 SUCCOA + 1 CYS + 1 MYTHF + 2 H_2O + 1 ATP → 1 MET + 1 COA + 1 SUC + 1 PYR + 1 NH_4 + 2 H + 1 ADP + 1 Pi + 1 THF

(74) 1 THR + 1 PYR + 1 NADPH + 1 GLUT + 2 H → 1 ILEU + NH_4 + 1 NADP + 1 H_2O + 1 CO_2 + 1 AKG

(75) 1 PRY + 1 GLUT → 1 ALA + 1 AKG

(76) 2 PYR + 1 NADPH + 2 H → 1 AKI + 1 CO_2 + 1 NADP + 1 H_2O

(77) 1 AKI + 1 GLUT → 1 VAL + 1 AKG

(78) 1 AKI + 1 ACCOA + 1 GLUT + 1 NAD + 2 H_2O + 1 ATP → 1 LEU + 1 AKG + 1 COA + 1 CO_2 + 2 H + 1 Pi + 1 NADH + 1 ADP

(79) 2 PEP + 1 E4P + 1 NADPH + 1 ATP → 1 CHO + 1 ADP + 4 Pi + 1 NADP

(80) 1 CHO + 1 GLUT + 1 H → 1 PHEN + 1 AKG + 1 CO_2 + 1 H_2O

(81) 1 CHO + 1 GLUT + 1 NAD → 1 TYR + 1 AKG + 1 CO_2 + 1 NADH

(82) 1 CHO + 1 GLUM + 1 PRPP + 1 SER → 1 TRYP + 2 Pi + 1 CO_2 + 1 GAP + 1 GLUT + 1 H + 1 PYR + 1 H_2O

(83) 1 RIBU5P + 2 ATP → 1 PRPP + 2 ADP + 1 H

(84) 1 PRPP + 3 ATP + 3 H_2O + 1 NH4 + 1 GLUM + 2 NAD + 1 NADPH + 1 CO_2 → 1 HIS + 6 Pi + 2 NADH + 1 NADP + 3 ADP + 1 AKG + 8 H

Amino acid polymerization

(85) 0.0820 GLUT + 0.0285 GLUM + 0.0448 PRO + 0.0437 ARG + 0.0776 LYS + 0.0502 SER + 0.0787 GLY + 0.0019 CYS + 0.0806 ASP + 0.0277 ASN + 0.0518 THR + 0.0138 MET + 0.0524 ILEU + 0.1246 ALA + 0.0719 VAL + 0.0803 LEU + 0.0364 PHEN + 0.0277 TYR + 0.0076 TRYP + 0.0179 HIS → 1 AM

(86) 1 AM + 4 ATP + 3 H_2O → 4.8248 PROT + 4 ADP + 4 H + 4 Pi

Nucleotide synthesis

(87) 1 PRPP + 2 GLUM + 1 GLY + 4 ATP + 1 ASP + 2 H_2O + 2 FTHF + 1 CO_2 → 1 IMP + 4 ADP + 6 Pi + 2 GLUT + 2 THF + 1 FUM + 8 H

(88) 1 IMP + 1 ASP + 1 ATP → 1 AMP + 1 ADP + 1 Pi + 1 FUM + 2 H

(89) 1 IMP + 1 NAD + 2 ATP + 1 GLUM + 3 H_2O → 1 GMP + 2 ADP + 2 Pi + 1 GLUT + 1 NADH + 4 H

(90) 1 GLUM + 1 PRPP + 2 ATP + 1 ASP + 2 H_2O + 1 NAD → 1 UMP + 2 ADP + 4 Pi + 1 GLUT + 1 NADH + 4 H

(91) 1 UMP + 2 ATP → 1 UTP + 2 ADP

(92) 1 UTP + 1 GLUM + 1 ATP + 1 H_2O → 1 CTP + 1 ADP + 1 Pi + 2 H + 1 GLUT

(93) 1 CTP + 2 ADP → 1 CMP + 2 ATP

RNA synthesis

(94) 0.2330 AMP + 0.2330 GMP + 0.3060 UMP + 0.2280 CMP + 3.2279 ATP + 2.2279 H_2O → 9.466 RNA + 3.22791 ADP + 3.22791 Pi + 3.22791 H

ATP consumption for maintenance

(95) 1 ATP + 1 H_2O → 1 ADP + 1 Pi + 1 H

Synthesis of fatty acids

(96) 8 ACCOA + 15 ATP + 15 NADPH + 1 O_2 + 7 H_2O → 1 PAL + 8 COA + 15 ADP + 15 NADP + 1 H + 15 Pi

(97) 9 ACCOA + 17 ATP + 17 NADPH + 1 O_2 + 8 H_2O → 1 OL + 9 COA + 17 ADP + 17 NADP + 1 H + 17 Pi

Synthesis of glycogen and polysaccharides

(98) 0.16667 GLUC6P + 0.16667 ATP + 0.16667 H_2O → 1 PSACH + 0.16667 ADP + 0.33333 Pi + 0.166667 H

Biomass formation

(99) 0.47003 PROT + 0.35376 PSACH + 0.05234 RNA + 0.00344 PAL + 0.00344 OL + 0.00266 GOH → 1 BIOM

NOMENCLATURE

C_i	concentration of compound i [(C)mol · L^{-1}]
D	dilution rate (h^{-1})
df	degree of freedom (−)
f	ethanol fraction of the feed (C-mol · C-mol^{-1} total carbon)
K	growth-associated maintenance coefficient (mol ATP · C-mol^{-1} biomass)
K'	growth-associated maintenance coefficient (mol ATP · C-mol^{-1} protein)
m_{ATP}	non-growth-associated maintenance coefficient (mol ATP · C-mol^{-1} biomass h^{-1})
m'_{ATP}	non-growth-associated maintenance coefficient (mol ATP · C-mol^{-1} protein h^{-1})
m	total number of compounds (−)
n	number of reactions (−)
p	number of compounds exchanged between the system and the environment (−)
q_i	specific conversion rate of compound i [(C)mol · C-mol^{-1} · h^{-1}]
$r_{A,i}$	net conversion rate of compound i [(C)mol · L^{-1} · h^{-1}]
r_j	volumetric rate of biochemical reaction j [(C)mol · L^{-1} · h^{-1}]
V	volume (L)
X_P	protein content of the biomass (C-mol · C-mol^{-1})
Y_{SP}	apparent yield of product on carbon substrate (C-mol · C-mol^{-1})
Y_{SP}^{lim}	limit to product yield on carbon substrate due to biochemical constraint (C-mol · C-mol^{-1})
Y_{SP}^{max}	product yield parameter in linear equation for consumption of carbon substrate (C-mol · C-mol^{-1})
Y_{SX}	apparent yield of biomass on carbon substrate (C-mol · C-mol^{-1})
Y_{SX}^{max}	biomass yield parameter in linear equation for consumption of carbon substrate (C-mol · C-mol^{-1})