

X_i Reaction

Glycolysis

- X₁ Glucose_{ext} + ATP => G6P + ADP
X₂ G6P <=> F6P
X₃ F6P + ATP => GAP + DHAP + ADP
X₄ GAP + 2ADP + NAD⁺ => Pyr + 2ATP + NADH
X₅ DHAP <=> GAP

Pentose Phosphate Pathway

- X₆ G6P + 2 NADP⁺ => RU5P + 2 NADPH + CO₂
X₇ RU5P <=> XU5P
X₈ RU5P <=> R5P
X₉ R5P + XU5P <=> S7P + GAP
X₁₀ E4P + XU5P <=> F6P + GAP
X₁₁ S7P + GAP <=> F6P + E4P

Pyruvate Dehydrogenase

- X₁₂ CoA + NAD⁺ + Pyr => AcCoA_{mit} + NADH + CO₂

TCA cycle

- X₁₃ AcCoA_{mit} + Oaa_{mit} => CoA + Cit_{mit}
X₁₄ Cit_{mit} + NAD⁺ => NADH + CO₂ + Akg_{mit}
X₁₅ NAD⁺ + Akg_{mit} + ADP + FAD => Mal + NADH + FADH₂ + ATP + CO₂
X₁₆ Mal + NAD⁺ => OAA_{mit} + NADH

Anaplerotic Pathways

- X₁₇ ATP + CO₂ + Pyr => Oaa_{cyt} + ADP

Fermentative Pathways

- X₁₈ Pyr => AcO + CO₂
X₁₉ AcO + NADP⁺ + CoA + ATP => NADPH + AcCoA_{cyt} + Pyrophosphate + AMP
X₂₀ AcO + NADH => Eth_{ext} + NAD⁺
X₂₁ DHAP + NADH + ATP => Glycerol_{cyt} + Orthophosphate + ADP + NAD⁺
X₂₂ XU5P + 2 NADH + NADP⁺ => ARA_{ext} + 2 NAD⁺ + NADPH

Cytosol-mitochondria transport reactions

- X₂₃ Oaa_{cyt} => Oaa_{mit} (in oxygen-limiting and hypoxic conditions)
X₂₃^{*} Oaa_{cyt} => Oaa_{mit} (in normoxic condition)

X₂₄ Oaa_{mit} => Oaa_{cyt} (in oxygen-limiting and hypoxic conditions)
X₂₅ Akg_{mit} => Akg_{cyt}

Metabolite excretion reactions

X₂₆ Glycerol_{cyt} => Glycerol_{ext}
X₂₇ Pyr => Pyr_{ext}
X₂₈ Cit => Cit_{ext}

Biomass synthesis reactions for each oxygenation condition

1. Protein (Composition derived from the amino acid composition of each oxygenation condition [18]).

X_{29.1} (21 % O₂ condition): 0.136 Pyr + 0.006 R5P + 0.013 E4P + 0.031 Oaa_{cyt} + 0.014
AcCoA_{mit} + 0.009 Oaa_{mit} + 0.075 Akg_{cyt} + 0.013 AcCoA_{cyt} + 0.300 NAD⁺ + 1.710 NADPH
=> 1 C-mol Protein + 0.002 GAP + 0.058 CO₂ + 0.300 NADH + 1.710 NADP⁺
X_{29.2} (11 % O₂ condition): 0.141 Pyr + 0.006 R5P + 0.013 E4P + 0.033 Oaa_{cyt} + 0.015
AcCoA_{mit} + 0.009 Oaa_{mit} + 0.070 Akg_{cyt} + 0.014 AcCoA_{cyt} + 0.303 NAD⁺ + 1.704 NADPH
=> 1 C-mol Protein + 0.002 GAP + 0.066 CO₂ + 0.303 NADH + 1.704 NADP⁺
X_{29.3} (8 % O₂ condition): 0.144 Pyr + 0.006 R5P + 0.014 E4P + 0.034 Oaa_{cyt} + 0.016
AcCoA_{mit} + 0.010 Oaa_{mit} + 0.068 Akg_{cyt} + 0.014 AcCoA_{cyt} + 0.239 NAD⁺ + 1.697 NADPH
=> 1 C-mol Protein + 0.002 GAP + 0.069 CO₂ + 0.239 NADH + 1.697 NADP⁺

2. Carbohydrate (Composition derived from [91])

X₃₀ 0.113 G6P + 0.053 F6P => 1 C-mol Carbohydrate

3. Glycogen

X₃₁ 0.166 G6P => 1 C-mol Glycogen

4. Lipid (Composition derived from the mean lipid composition of all conditions [18]).

X₃₂ 0.002 G6P + 0.005 Pyr + 0.006 CO₂ + 0.061 AcCoA_{mit} + 0.386 AcCoA_{cyt} + 0.065 O₂ +
0.022 Glycerol_{cyt} + 0.06 NADH + 0.77 NADPH => 1 C-mol Lipid + 0.06 NAD⁺ + 0.77
NADP⁺

5. RNA (Composition derived from the RNA composition proposed by [92])

X₃₃ 0.060 Pyr + 0.060 CO₂ + 0.111 R5P + 0.051 Oaa_{cyt} + 0.181 NAD⁺ + 0.079 NADPH => 1
C-mol RNA + 0.181 NADH + 0.079 NADP⁺

6. DNA (Composition derived from the DNA composition published in [31])

X₃₄ 0.054 Pyr + 0.085 CO₂ + 0.108 R5P + 0.054 Oaa_{cyt} + 0.161 NAD⁺ + 0.225 NADPH => 1
C-mol DNA + 0.161 NADH + 0.225 NADP⁺