

Reaction Details

Reactions involved in the loop in the yeast GSMR:

- ACONTm: [m] Citrate \rightleftharpoons Isocitrate
- OAA2m: [c] Citrate \rightleftharpoons Isocitrate
- CITtem: Citrate⁻³[c] + Isocitrate⁻³[m] \rightleftharpoons Citrate⁻³[m] + Isocitrate⁻³[c]

Reactions constituting the PC in LH sampling of the yeast GSMR:

- NADH2-u6m[m]: H⁺ + NADH + Ubiquinone \rightarrow NAD⁺ + Ubiquinol
- NADH2-u6c: H⁺[c] + NADH[c] + Ubiquinone[m] \rightarrow NAD⁺[c] + Ubiquinol[m]
- ALCD2x[c]: Ethanol + NAD⁺ \rightleftharpoons Acetaldehyde + H⁺ + NADH
- ALCD2m[m]: Ethanol + NAD⁺ \rightleftharpoons Acetaldehyde + H⁺ + NADH
- ETOHtm: Ethanol[c] \rightleftharpoons Ethanol[m]
- ACALDtm: Acetaldehyde [c] \rightleftharpoons Acetaldehyde [m]

Reactions involved in loops in *Pseudomonas aeruginosa* GSMR (iMO1086):

- RR10392: NAD⁺ + L-Isoleucine + H₂O \rightleftharpoons (S)-3-Methyl-2-oxopentanoate + H⁺ + NH₄⁺ + NADH
- RR08749: L-Glutamate[e] + H⁺[e] \rightleftharpoons H⁺ + L-Glutamate
- RR08696: Sodium + H⁺[e] \rightleftharpoons Sodium[e] + H⁺
- RR04305: L-Glutamate + NADP⁺ + H₂O \rightleftharpoons H⁺ + NADPH + NH₄⁺
- RR03658: NAD⁺ + L-Valine + H₂O \rightleftharpoons 3-Methyl-2-oxobutanoate + 2-Oxoglutarate + H⁺ + NH₄⁺ + NADH
- RR02406: 10-Formyltetrahydrofolate + 5'-Phosphoribosylglycinamide \rightleftharpoons H⁺ + Tetrahydrofolate + 5'-Phosphoribosyl-N-formylglycinamide
- RR01210: L-Isoleucine + 2-Oxoglutarate \rightleftharpoons (S)-3-Methyl-2-oxopentanoate + L-Glutamate
- RR00902: 5,10-Methenyltetrahydrofolate + H₂O \rightleftharpoons 10-Formyltetrahydrofolate
- RR00767: L-Valine + 2-Oxoglutarate \rightleftharpoons 3-Methyl-2-oxobutanoate + L-Glutamate
- RR00710: L-Leucine + 2-Oxoglutarate \rightleftharpoons 4-Methyl-2-oxopentanoate + L-Glutamate
- RR00708: NAD⁺ + L-Leucine + H₂O \rightleftharpoons 4-Methyl-2-oxopentanoate + H⁺ + NH₄⁺ + NADH

- RR00703: (S)-Malate \rightleftharpoons Fumarate + H₂O
- RR00563: 2-Oxoglutarate + beta-Alanine \rightleftharpoons 3-Oxopropanoate + L-Glutamate
- RR00562: L-Alanine + 3-Oxopropanoate \rightleftharpoons Pyruvate + beta-Alanine
- RR00191: 2-Oxoglutarate + L-Aspartate \rightleftharpoons Oxaloacetate + L-Glutamate
- RR00179: NAD⁺ + (S)-Malate + NADH \rightleftharpoons Oxaloacetate + H⁺
- RR00079: NAD⁺ + NADPH \rightleftharpoons NADH + NADP⁺
- RR00124: L-Alanine + 2-Oxoglutarate \rightleftharpoons Pyruvate + L-Glutamate
- IR02407: 5,10-Methenyltetrahydrofolate + 5'-Phosphoribosylglycinamide + H₂O \rightarrow H⁺ + Tetrahydrofolate + 5'-Phosphoribosyl-N-formylglycinamide
- IR00255: L-Aspartate \rightarrow Fumarate + NH₄⁺
- IR08751: Sodium[e] + L-Glutamate[e] \rightarrow Sodium + L-Glutamate
- RR10079: H⁺[e] + Citrate[e] \rightleftharpoons Citrate + H⁺
- RR10072: Magnesium \rightleftharpoons Magnesium[e]
- IR09937: Magnesium[e] + H⁺[e] + Citrate[e] \rightarrow Citrate + H⁺ + Magnesium

Reactions involved in loops in iMO1086 to which constraints were applied (Flux value reduced to zero):

- RR10392
- RR10072
- RR08696
- RR04305
- RR00767
- RR00124
- IR09937
- IR08751
- IR02407

Reactions constituting the PCs in iM1086

PC1:

- RR00448: Ethanol + NAD⁺ \rightleftharpoons Acetaldehyde + H⁺ + NADH
- IR02668: Ethanol + PQQ \rightarrow Acetaldehyde + PQQH₂

- IR10115: Ubiquinone-8 + H⁺ + PQQH₂ → H⁺[e] + Ubiquinol-8 + PQQ
- IR08605: Ubiquinone-8 + H⁺ + NADH → NAD⁺ + H⁺[e] + Ubiquinol-8

PC 2:

- RR00216: Succinate + ATP + CoA <=> Succinyl-CoA + Orthophosphate + ADP
- RR00079: NAD⁺ + NADPH <=> NADH + NADP⁺
- IR03527: NAD⁺ + Pyruvate + CoA → Acetyl-CoA + NADH
- RR00179: NAD⁺ + (S)-Malate <=> Oxaloacetate + H⁺ + NADH
- IR00244: Isocitrate <=> Succinate + Glyoxylate
- IR04615: Acetyl-CoA + Glyoxylate + H₂O → H⁺ + CoA + (S)-Malate
- RR00131: Isocitrate + NADP⁺ <=> NADPH + 2-Oxoglutarate + CO₂
- IR08963: NAD⁺ + CoA + 2-Oxoglutarate → Succinyl-CoA + NADH + CO₂
- RR00181: HCO₃⁻ + Pyruvate + ATP <=> Orthophosphate + Oxaloacetate + H⁺ + ADP
- RR08916: CO₂ + H₂O <=> HCO₃⁻ + H⁺

PC3:

- IR09309: H⁺ + NADPH + 6-Phospho-2-dehydro-D-gluconate → 6-Phospho-D-gluconate + NADP⁺
- IR09308: 2-dehydro-D-gluconate + ATP → H⁺ + ADP + 6-Phospho-2-dehydro-D-gluconate
- IR09593: 2-dehydro-D-gluconate[e] + H⁺[e] → 2-dehydro-D-gluconate + H⁺
- IR09306: D-Gluconic acid[e] + NADP⁺ → 2-Dehydro-D-gluconate[e] + H⁺ + NADPH
- IR00962: ATP + D-Gluconic acid → H⁺ + ADP + 6-Phospho-D-gluconate
- IR08758: D-Gluconic acid[e] + H⁺[e] → H⁺ + D-Gluconic acid

PC 4:

- RR03591: ATP + dADP <=> dATP + ADP
- IR07969: H⁺ + dADP + Phosphoenolpyruvate → dATP + Pyruvate
- RR01038: ATP + dGDP <=> ADP + dGTP
- IR05416: H⁺ + Phosphoenolpyruvate + dGDP → Pyruvate + dGTP

PC 5:

- RR03591: ATP + dADP <=> dATP + ADP
- IR07969: H⁺ + dADP + Phosphoenolpyruvate → dATP + Pyruvate
- IR05416: H⁺ + Phosphoenolpyruvate + dGDP → Pyruvate + dGTP

- RR01038: $\text{ATP} + \text{dGDP} \rightleftharpoons \text{ADP} + \text{dGTP}$
- RR00170: $\text{ATP} + \text{GDP} \rightleftharpoons \text{ADP} + \text{GTP}$
- IR07938: $\text{H}^+ + \text{Phosphoenolpyruvate} + \text{GDP} \rightarrow \text{Pyruvate} + \text{GTP}$
- IR04559: $\text{Phosphoenolpyruvate} + \text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{Orthophosphate} + \text{Oxaloacetate}$
- RR00181: $\text{HCO}_3^- + \text{Pyruvate} + \text{ATP} \rightleftharpoons \text{Orthophosphate} + \text{Oxaloacetate}$
- RR08916: $\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{HCO}_3^- + \text{H}^+$

PC 6:

- RR08916: $\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{HCO}_3^- + \text{H}^+$
- RR00170: $\text{ATP} + \text{GDP} \rightleftharpoons \text{ADP} + \text{GTP}$
- IR07938: $\text{H}^+ + \text{Phosphoenolpyruvate} + \text{GDP} \rightarrow \text{Pyruvate} + \text{GTP}$
- IR04559: $\text{Phosphoenolpyruvate} + \text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{Orthophosphate} + \text{Oxaloacetate}$
- RR00181: $\text{HCO}_3^- + \text{Pyruvate} + \text{ATP} \rightleftharpoons \text{Orthophosphate} + \text{Oxaloacetate}$

PC7:

- RR00181: $\text{HCO}_3^- + \text{Pyruvate} + \text{ATP} \rightleftharpoons \text{Orthophosphate} + \text{Oxaloacetate}$
- RR03591: $\text{ATP} + \text{dADP} \rightleftharpoons \text{dATP} + \text{ADP}$
- RR00170: $\text{ATP} + \text{GDP} \rightleftharpoons \text{ADP} + \text{GTP}$
- RR08916: $\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{HCO}_3^- + \text{H}^+$
- RR01038: $\text{ATP} + \text{dGDP} \rightleftharpoons \text{ADP} + \text{dGTP}$
- IR07938: $\text{H}^+ + \text{Phosphoenolpyruvate} + \text{GDP} \rightarrow \text{Pyruvate} + \text{GTP}$
- IR07898: $\text{H}^+ + \text{Phosphoenolpyruvate} + \text{ADP} \rightarrow \text{Pyruvate} + \text{ATP}$
- IR07969: $\text{H}^+ + \text{Phosphoenolpyruvate} + \text{dADP} \rightarrow \text{dATP} + \text{Pyruvate}$
- IR05416: $\text{H}^+ + \text{Phosphoenolpyruvate} + \text{dGDP} \rightarrow \text{Pyruvate} + \text{dGTP}$
- IR04559: $\text{Phosphoenolpyruvate} + \text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{Orthophosphate} + \text{Oxaloacetate}$