

## Electronic Supplementary Information (ESI) for Molecular BioSystems

### Genome-scale metabolic network analysis and drug targeting of multi-drug resistant pathogen *Acinetobacter baumannii* AYE

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**Supplementary Table 1.** Metabolic reactions of AbyMBEL891 with information on their genes and enzymes.

**Supplementary Table 2.** Metabolites participating in reactions of AbyMBEL891.

**Supplementary Table 3.** Biomass composition of *Acinetobacter baumannii*.

**Supplementary Table 4.** List of 246 essential reactions predicted under minimal medium with succinate as a sole carbon source.

**Supplementary Table 5.** List of 681 reactions considered for comparison of their essentiality in AbyMBEL891 with those from *Acinetobacter baylyi* ADP1.

**Supplementary Table 6.** List of 162 essential reactions predicted under arbitrary complex medium.

**Supplementary Table 7.** List of 211 essential metabolites predicted under arbitrary complex medium.

#### **AbyMBEL891.sbml**

Genome-scale metabolic model of *Acinetobacter baumannii* AYE, AbyMBEL891, is available as a separate file in the format of Systems Biology Markup Language (SBML) version 2.

**Supplementary Table 1.** Metabolic reactions of AbyMBEL891 with information on their genes and enzymes. Highlighted (yellow) reactions indicate that they are not assigned with genes.

| No.  | Metabolism                               | EC Number | ORF   | Reaction                               | Enzyme   |
|------|--|-----------|---|--|--|
| R001 | Glycolysis/ Gluconeogenesis              | 5.1.3.3   | ABAYE2829   | GLC <-> bDGLC                          | aldose 1-epimerase   |
| R002 | Glycolysis/ Gluconeogenesis              | 5.3.1.9   | ABAYE3801   | G6P <-> bDG6P                          | glucose-6-phosphate isomerase  |
| R003 | Glycolysis/ Gluconeogenesis              | 5.3.1.9   | ABAYE3801   | G6P <-> F6P                            | glucose-6-phosphate isomerase  |
| R004 | Glycolysis/ Gluconeogenesis              | 5.3.1.9   | ABAYE3801   | bDG6P <-> F6P                          | glucose-6-phosphate isomerase  |
| R005 | Glycolysis/ Gluconeogenesis              | 5.4.2.2   | ABAYE2928 OR ABAYE3800  | G6P <-> G1P                            | phosphoglucomutase OR phosphomannomutase   |
| R006 | Glycolysis/ Gluconeogenesis              | 3.1.3.11  | ABAYE0899   | FDP -> F6P + PI                        | fructose-1,6-bisphosphatase  |
| R007 | Glycolysis/ Gluconeogenesis              | 4.1.2.13  | ABAYE2088   | FDP <-> G3P + DHAP                     | fructose-1,6-bisphosphate aldolase   |
| R008 | Glycolysis/ Gluconeogenesis              | 5.3.1.1   | ABAYE3443   | DHAP <-> G3P                           | triosephosphate isomerase  |
| R009 | Glycolysis/ Gluconeogenesis              | 1.2.1.12  | ABAYE0958   | G3P + PI + NAD <-> NADH + 13PDG        | glyceraldehyde 3-phosphate dehydrogenase   |
| R010 | Glycolysis/ Gluconeogenesis              | 2.7.2.3   | ABAYE2090   | 13PDG + ADP <-> 3PG + ATP              | phosphoglycerate kinase  |
| R011 | Glycolysis/ Gluconeogenesis              | 5.4.2.1   | ABAYE3537   | 3PG <-> 2PG                            | phosphoglycerate mutase  |
| R012 | Glycolysis/ Gluconeogenesis              | 4.2.1.11  | ABAYE1669   | 2PG <-> PEP                            | enolase  |
| R013 | Glycolysis/ Gluconeogenesis              | 2.3.1.12  | ABAYE0158 OR ABAYE1946  | COA + ADLIPO -> DLIPO + ACCOA          | pyruvate dehydrogenase E2 component (dihydrolipoamideacetyltransferase)                      |
| R014 | Glycolysis/ Gluconeogenesis              | 1.8.1.4   | ABAYE0505 OR ABAYE0782 OR ABAYE1945   | DLIPO + NAD -> LIPO + NADH             | dihydrolipoamide dehydrogenase   |
| R015 | Glycolysis/ Gluconeogenesis              | 6.2.1.1   | ABAYE0179 OR ABAYE1413 OR ABAYE3766   | ATP + AC + COA <-> AMP + PPI + ACCOA   | acetyl-CoA synthetase  |
| R016 | Glycolysis/ Gluconeogenesis              | 1.2.1.3   | ABAYE1028 OR ABAYE1460 OR ABAYE2333 OR ABAYE2837  | ACAL + NAD -> NADH + AC                | aldehyde dehydrogenase   |
| R017 | Glycolysis/ Gluconeogenesis              | 1.1.1.1   | ABAYE0763 OR ABAYE1463 OR ABAYE1522 OR ABAYE1861 OR p2ABAYE0004 OR p3ABAYE0020 OR p3ABAYE0024   | ACAL + NADH <-> ETH + NAD              | alcohol dehydrogenase  |
| R018 | Glycolysis/ Gluconeogenesis              | 4.1.1.1   | ABAYE1030   | ACAL + THMPP <-> 2(HE)TPP              | pyruvate decarboxylase/indolepyruvate decarboxylase  |
| R019 | TCA cycle                                | 2.3.3.1   | ABAYE0773   | ACCOA + OA -> COA + CIT                | citrate synthase   |
| R020 | TCA cycle                                | 4.2.1.3   | ABAYE1432 OR ABAYE3228 OR ABAYE3791   | CIT <-> ICIT                           | aconitate hydratase  |
| R021 | TCA cycle                                | 1.1.1.42  | ABAYE0980 OR ABAYE0982  | ICIT + NADP -> NADPH + AKG + CO2       | isocitrate dehydrogenase   |
| R022 | TCA cycle                                | 1.2.4.2   | ABAYE0780   | AKG + LIPO -> SDLIPO + CO2             | 2-oxoglutarate dehydrogenase E1 component  |
| R023 | TCA cycle                                | 2.3.1.61  | ABAYE0781   | SDLIPO + COA -> DLIPO + SUCCOA         | 2-oxoglutarate dehydrogenase E2 component  |
| R024 | TCA cycle                                | 6.2.1.5   | ABAYE0783 AND ABAYE0784   | ADP + PI + SUCCOA <-> ATP + SUCC + COA | succinyl-CoA synthetase  |
| R025 | TCA cycle                                | 1.3.99.1  | ABAYE0774 AND ABAYE0775 AND ABAYE0776 AND ABAYE0777   | SUCC + FAD -> FUM + FADH2              | succinate dehydrogenase  |
| R026 | TCA cycle                                | 1.3.99.1  | ABAYE0774 AND ABAYE0775 AND ABAYE0776 AND ABAYE0777   | FUM + MKH2 -> SUCC + MK                | fumarate reductase   |
| R027 | TCA cycle                                | 1.3.99.1  | ABAYE0774 AND ABAYE0775 AND ABAYE0776 AND ABAYE0777   | FUM + DMKH2 -> SUCC + DMK              | fumarate reductase   |
| R028 | TCA cycle                                | 4.2.1.2   | ABAYE1563 OR ABAYE3284  | FUM <-> MAL                            | fumarate hydratase   |
| R029 | TCA cycle                                | 1.1.1.37  | ABAYE0465   | MAL + NAD <-> NADH + OA                | malate dehydrogenase   |
| R030 | Pentose phosphate pathway                | 5.1.3.1   | ABAYE3114   | RL5P <-> X5P                           | D-ribose-5-phosphate 3-epimerase   |
| R031 | Pentose phosphate pathway                | 5.3.1.6   | ABAYE1650   | RL5P <-> R5P                           | ribose 5-phosphate isomerase A   |
| R032 | Pentose phosphate pathway                | 2.2.1.1   | ABAYE2116 OR (ABAYE2823 AND ABAYE2824)  | R5P + X5P <-> G3P + S7P                | transketolase  |
| R033 | Pentose phosphate pathway                | 2.2.1.1   | ABAYE2116 OR (ABAYE2823 AND ABAYE2824)  | X5P + E4P <-> F6P + G3P                | transketolase  |
| R034 | Pentose phosphate pathway                | 2.2.1.2   | ABAYE1510   | G3P + S7P <-> E4P + F6P                | transaldolase  |
| R035 | Pentose phosphate pathway                | 4.1.2.4   |   | DR5P -> G3P + ACAL                     | deoxyribose-phosphate aldolase   |
| R036 | Pentose phosphate pathway                | 5.4.2.7   |   | DR1P <-> DR5P                          | phosphopentomutase   |
| R037 | Pentose phosphate pathway                | 4.1.2.14  | ABAYE3280   | KDPG -> PYR + G3P                      | bifunctional 4-hydroxy-2-oxoglutarate aldolase OR 2-dehydro-3-deoxyphosphogluconate aldolase |
| R038 | Pentose phosphate pathway                | 2.7.1.12  | ABAYE3278   | GLUC + ATP -> D6PGC + ADP              | gluconokinase  |
| R039 | Pentose phosphate pathway                | 4.2.1.12  | ABAYE3281   | D6PGC -> KDPG                          | phosphogluconate dehydratase   |
| R040 | Pentose phosphate pathway                | 5.4.2.2   | ABAYE2928 OR ABAYE3800  | R1P <-> R5P                            | phosphoglucomutase OR phosphomannomutase   |
| R041 | Pentose and glucuronate interconversions | 1.1.1.22  | ABAYE3802   | UDPG + 2 NAD <-> UDPGLUC + 2 NADH      | UDP-glucose 6-dehydrogenase  |
| R042 | Fructose and mannose metabolism          | 2.7.1.56  | ABAYE1613   | F1P + ATP -> FDP + ADP                 | fructose-1-phosphate kinase  |
| R043 | Fructose and mannose metabolism          | 4.1.2.13  | ABAYE2088   | F1P -> DHAP + T3                       | fructose-bisphosphate aldolase   |
| R044 | Fructose and mannose metabolism          | 5.3.1.8   |   | MAN6P <-> F6P                          | phosphomannose isomerase   |
| R045 | Fructose and mannose metabolism          | 5.4.2.8   | ABAYE2928 OR ABAYE3800  | MAN6P <-> MAN1P                        | phosphomannomutase   |
| R046 | Fructose and mannose metabolism          | 2.7.7.13  |   | GTP + MAN1P <-> PPI + GDPMAN           | nucleoside-diphosphate-sugar pyrophosphorylase   |
| R047 | Fructose and mannose metabolism          | 1.1.1.-   | ABAYE0043 OR ABAYE0109 OR ABAYE0479 OR ABAYE1356 OR ABAYE2589 OR ABAYE2607 OR ABAYE2613 OR ABAYE2618 OR ABAYE2845 OR ABAYE3187 OR ABAYE3378 | S6P + NADP <-> SB1P + NADPH            | alcohol dehydrogenase  |

| No.  | Metabolism                              | EC Number            | ORF   | Reaction                               | Enzyme   |
|------|---|----------------------|---|--|--|
| R048 | Fructose and mannose metabolism         | 4.1.2.17             | ABAYE3670   | FUCP <=> DHAP + LACAL                  | aldolase class II  |
| R049 | Galactose metabolism                    | 5.1.3.2              | ABAYE1562 OR ABAYE3804  | UDPG <=> UDPGAL                        | UDP-glucose 4-epimerase  |
| R050 | Galactose metabolism                    | 2.7.7.9              | ABAYE3803   | G1P + UTP <=> UDPG + PPI               | UTP-glucose-1-phosphate uridylyltransferase                                      |
| R051 | Ascorbate and aldarate metabolism       | 1.2.1.3              | ABAYE1028 OR ABAYE1460 OR ABAYE2333 OR ABAYE2837              | DGLUCL + NAD <=> DGLUCA + NADH         | aldehyde dehydrogenase   |
| R052 | Starch and sucrose metabolism           | 3.2.1.93             |   | TRE6P -> GLC + G6P                     | trehalose-6-phosphate hydrolase  |
| R053 | Starch and sucrose metabolism           | 2.4.1.15             | ABAYE3007   | UDPG + G6P <=> UDP + TRE6P             | trehalose-6-phosphate synthase   |
| R054 | Starch and sucrose metabolism           | 3.1.3.12             | ABAYE3006   | TRE6P -> TRE + PI                      | trehalose-6-phosphate phosphatase, biosynthetic                                  |
| R055 | Aminosugars metabolism                  | 2.6.1.16             | ABAYE0089   | F6P + GLN -> GLU + GA6P                | glucosamine-fructose-6-phosphate aminotransferase                                |
| R056 | Aminosugars metabolism                  | 5.4.2.10             | ABAYE0167   | GA6P <=> GA1P                          | phosphomannomutase   |
| R057 | Aminosugars metabolism                  | 2.3.1.157            | ABAYE0090   | ACCOA + GA1P -> NAGA1P + COA           | glucosamine-1-phosphate N-acetyltransferase                                      |
| R058 | Aminosugars metabolism                  | 2.7.7.23             | ABAYE0090   | UTP + NAGA1P <=> UDPNAG + PPI          | UDP-N-acetylglucosamine pyrophosphorylase  |
| R059 | Aminosugars metabolism                  | 5.1.3.14             | ABAYE0969   | UDPNAG <=> NADMA + UDP                 | UDP-N-acetylglucosamine 2-epimerase  |
| R060 | Aminosugars metabolism                  | 5.1.3.14             | ABAYE0969   | UDPNAG <=> UDPNADMA                    | UDP-N-acetylglucosamine 2-epimerase  |
| R061 | Aminosugars metabolism                  | 1.1.1.-              | ABAYE3815   | UDPNADMA + 2 NAD -> UDPNADMAU + 2 NADH | UDP-N-acetyl-D-mannosaminuronate dehydrogenase                                   |
| R062 | Aminosugars metabolism                  | 2.5.1.7              | ABAYE3133   | UDPNAG + PEP -> UDPNAGEP + PI          | UDP-N-acetylglucosamine enolpyruvyl transferase                                  |
| R063 | Aminosugars metabolism                  | 1.1.1.158            | ABAYE1526   | UDPNAGEP + NADPH -> UDPNAM + NADP      | UDP-N-acetylenolpyruvoylglucosamine reductase                                    |
| R064 | Aminosugars metabolism                  | 3.2.1.-              | ABAYE2663   | GLCAMN <=> GLCA + GLCAMN               | bifunctional protein [includes: lytic murein transglycosylase C, membrane-bound  |
| R065 | Aminosugars metabolism                  | 3.2.1.52             | ABAYE3272   | CHITB -> 2 NAGA                        | beta-N-acetyl-D-glucosaminidase  |
| R066 | Aminosugars metabolism                  | 5.1.3.7              | ABAYE3814   | UDPNAG <=> UDPAGLACA                   | NAD-dependent epimerase/dehydratase  |
| R067 | Nucleotide sugars metabolism            | 5.1.3.2              | ABAYE1562 OR ABAYE3804  | DTDPGLU <=> DTDPGLAC                   | UDP-glucose 4-epimerase  |
| R068 | Nucleotide sugars metabolism            | 2.7.7.24             |   | G1P + DTPP -> DTDPGLU + PPI            | glucose-1-phosphate thymidyltransferase  |
| R069 | Nucleotide sugars metabolism            | 4.2.1.46             |   | DTDPGLU -> DTDP4O6DG                   | dTDP-glucose 4,6 dehydratase   |
| R070 | Nucleotide sugars metabolism            | 5.1.3.13             |   | DTDP4O6DG -> DTDP4ORMNS                | dTDP-4-deoxyribose-3,5-epimerase   |
| R071 | Nucleotide sugars metabolism            | 1.1.1.133            |   | DTDP4ORMNS + NADPH -> DTDP4RMNS + NADP | dTDP-4-dehydroribose reductase   |
| R072 | Pyruvate metabolism                     | 2.7.9.2              | ABAYE1391   | ATP + PYR -> AMP + PEP + PI            | phosphoenolpyruvate synthase   |
| R073 | Pyruvate metabolism                     | 1.1.1.28             | ABAYE3796   | PYR + NADH <=> LAC + NAD               | D-lactate dehydrogenase  |
| R074 | Pyruvate metabolism                     | 2.3.1.8              | ABAYE1138 OR ABAYE3283  | ACCOA + PI <=> ACETYLP + COA           | phosphate acetyltransferase  |
| R075 | Pyruvate metabolism                     | 6.2.1.1              | ABAYE0179 OR ABAYE1413 OR ABAYE3766                           | AAD + COA <=> AMP + ACCOA              | acetyl-CoA synthase  |
| R076 | Pyruvate metabolism                     | 6.2.1.1              | ABAYE0179 OR ABAYE1413 OR ABAYE3766                           | ATP + AC <=> PPI + AAD                 | acetyl-CoA synthetase  |
| R077 | Pyruvate metabolism                     | 2.7.2.1              | ABAYE3282   | ACETYLP + ADP <=> AC + ATP             | acetate kinase   |
| R078 | Pyruvate metabolism                     | 4.1.1.31             | ABAYE0028   | PEP + CO2 -> OA + PI                   | phosphoenolpyruvate carboxylase  |
| R079 | Pyruvate metabolism                     | 1.1.1.38 OR 1.1.1.40 | ABAYE3731 OR ABAYE1138  | MAL + NAD <=> PYR + CO2 + NADH         | malate dehydrogenase   |
| R080 | Pyruvate metabolism                     | 1.1.1.38 OR 1.1.1.40 | ABAYE3731 OR ABAYE1138  | MAL + NADP <=> PYR + CO2 + NADPH       | malate dehydrogenase   |
| R081 | Pyruvate metabolism                     | 2.3.3.9              | ABAYE2053   | ACCOA + GLX -> MAL + COA               | malate synthase  |
| R082 | Pyruvate metabolism                     | 2.3.1.9              | ABAYE0629 OR ABAYE0638 OR ABAYE1916 OR ABAYE2307              | 2 ACCOA -> COA + AACCOA                | acetyl-CoA acetyltransferase   |
| R083 | Pyruvate metabolism                     | 4.4.1.5              | ABAYE1052   | RGT + MTG <=> LTG                      | lactoylglutathione lyase   |
| R084 | Pyruvate metabolism                     | 3.1.2.6              | ABAYE1362 OR ABAYE1940  | LTG -> RGT + LAC                       | hydroxyacylglutathione hydrolase GloB  |
| R085 | Pyruvate metabolism                     | 1.1.2.3              | ABAYE3797   | SLAC + 2 FERIC <=> PYR + 2 FEROC       | L-lactate dehydrogenase, FMN linked  |
| R086 | Pyruvate metabolism                     | 1.1.99.16            | ABAYE2869   | MAL + FAD -> FADH2 + OA                | malate dehydrogenase   |
| R087 | Pyruvate metabolism                     | 1.2.1.3              | ABAYE1028 OR ABAYE1460 OR ABAYE2333 OR ABAYE2837              | ACAL + NADP <=> AC + NADPH             | aldehyde dehydrogenase   |
| R088 | Pyruvate metabolism                     | 1.2.4.1              | ABAYE0157 OR (ABAYE1947 AND ABAYE1948)                        | 2(HE)TTP + LIPO <=> ADLIPO + THMPP     | pyruvate dehydrogenase subunit E1  |
| R089 | Pyruvate metabolism                     | 2.3.3.13             | ABAYE3292   | IPPAL + COA <=> ACCOA + OIVAL          | 2-isopropylmalate synthase   |
| R090 | Pyruvate metabolism                     | 4.1.1.-              | ABAYE1027   | PYR + CO2 <=> HEDC                     | L-2,4-diaminobutyrate decarboxylase  |
| R091 | Pyruvate metabolism                     | 4.1.1.32             | ABAYE0818   | GTP + OA <=> GDP + PEP + CO2           | phosphoenolpyruvate carboxylase [GTP] (PEP                                       |
| R092 | Pyruvate metabolism                     | 4.1.1.32             | ABAYE0818   | ITP + OA <=> IDP + PEP + CO2           | phosphoenolpyruvate carboxylase [GTP] (PEP carboxylase)                          |
| R093 | Glyoxylate and dicarboxylate metabolism | 4.1.3.1              | ABAYE2783   | ICIT -> SUCC + GLX                     | isocitrate lyase   |
| R094 | Glyoxylate and dicarboxylate metabolism | 1.2.1.2              | ABAYE0850   | FORMATE + NAD -> CO2 + NADH            | formate dehydrogenase  |
| R095 | Glyoxylate and dicarboxylate metabolism | 1.2.1.21             |   | GLAL + NAD -> NADH + GLYCOLATE         | glycolaldehyde dehydrogenase   |
| R096 | Glyoxylate and dicarboxylate metabolism | 3.1.3.18             | ABAYE0081 OR ABAYE2988 OR ABAYE3373 OR ABAYE3498 OR ABAYE3835 | 2PPG -> GLYCOLATE + PI                 | phosphoglycolate phosphatase   |
| R097 | Glyoxylate and dicarboxylate metabolism | 1.1.1.60             | ABAYE1786   | DGLYCERATE + NAD <=> HOPP + NADH       | 2-hydroxy-3-oxopropionate reductase OR tartronate semialdehyde reductase         |
| R098 | Glyoxylate and dicarboxylate metabolism | 1.1.1.60             | ABAYE1786   | DGLYCERATE + NADP <=> HOPP + NADPH     | 2-hydroxy-3-oxopropionate reductase OR tartronate semialdehyde reductase         |
| R099 | Glyoxylate and dicarboxylate metabolism | 1.1.1.93             | ABAYE2964   | MTTA + NAD <=> 2H3OSUCC + NADH         | tartrate dehydrogenase/decarboxylase OR D-malate dehydrogenase [decarboxylating] |
| R100 | Glyoxylate and dicarboxylate metabolism | 1.1.1.93             | ABAYE2964   | TTA + NAD <=> 2H3OSUCC + NADH          | tartrate dehydrogenase/decarboxylase OR D-malate dehydrogenase [decarboxylating] |
| R101 | Glyoxylate and dicarboxylate metabolism | 2.3.3.9              | ABAYE2053   | MAL + COA <=> ACCOA + GLX              | malate synthase G  |
| R102 | Glyoxylate and dicarboxylate metabolism | 5.3.1.22             | ABAYE3188   | HPYR <=> HOPP                          | hydroxypyruvate isomerase  |

| No.  | Metabolism                                      | EC Number                           | ORF   | Reaction                                   | Enzyme   |
|------|---|-------------------------------------|---|--|--|
| R103 | Propanoate metabolism                           | 4.2.1.17                            | ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3763 OR<br>ABAYE3764 OR<br>ABAYE3470 | 3HPCOA <-> PPCOA                           | enoyl-CoA hydratase/isomerase OR 3-methylglutaconyl-CoA hydratase                |
| R104 | Propanoate metabolism                           | 6.2.1.1                             | ABAYE0179 OR<br>ABAYE1413 OR<br>ABAYE3766   | ATP + PROPANOATE <-> PPI + PPA             | acetyl-CoA synthetase  |
| R105 | Propanoate metabolism                           | 6.2.1.1                             | ABAYE0179 OR<br>ABAYE1413 OR<br>ABAYE3766   | PPA + COA <-> AMP + PPACOA                 | propionyl-CoA synthetase   |
| R106 | Propanoate metabolism                           | 2.7.2.1                             | ABAYE3282   | PROPANOATE + ATP <-> PROPIONYL P + ADP     | acetate kinase   |
| R107 | Propanoate metabolism                           | 2.3.1.8                             | ABAYE1138 OR<br>ABAYE3283   | PPACOA + PI <-> PROPIONYL P + COA          | phosphate acetyltransferase  |
| R108 | Propanoate metabolism                           | 2.3.1.54                            |   | OBUT + COA <-> PPACOA + FORMATE            | formate acetyltransferase  |
| R109 | Propanoate metabolism                           | 1.2.1.3                             | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | 2P1A + NAD -> PPN + NADH                   | aldehyde dehydrogenase   |
| R110 | Propanoate metabolism                           | 2.3.3.5                             | ABAYE3792   | 2MCIT + COA <-> PPACOA + OA                | 2-methylcitrate synthase   |
| R111 | Propanoate metabolism                           | 4.1.3.30                            | ABAYE3793   | 3HB123TC <-> PYR + SUCC                    | methylisocitrate lyase   |
| R112 | Propanoate metabolism                           | 1.2.1.27                            | ABAYE1296 OR<br>ABAYE3768   | MMSA + COA + NAD -> PPACOA + CO2 + NADH    | methylmalonate-semialdehyde dehydrogenase  |
| R113 | Propanoate metabolism                           | 1.3.99.3                            | ABAYE0476 OR<br>ABAYE2013   | PPACOA + FAD <-> FADH2 + PPCOA             | acyl-CoA dehydrogenase   |
| R114 | Propanoate metabolism                           | 4.1.1.4                             | ABAYE1742   | AAC -> ACTN + CO2                          | acetoacetate decarboxylase   |
| R115 | Propanoate metabolism                           | 6.4.1.3                             | ABAYE0480   | ATP + PPACOA + HCO3 <-> ADP + PI + MMALCOA | propionyl-CoA carboxylase  |
| R116 | Glycolysis/Gluconeogenesis/Butanoate metabolism | 2.2.1.6 OR<br>4.1.1.1 OR<br>1.2.4.1 | (ABAYE2836 OR<br>ABAYE3239 OR<br>ABAYE3240) OR<br>ABAYE1030 OR<br>ABAYE0157 OR<br>(ABAYE1947 AND<br>ABAYE1948)  | THMPP + PYR -> 2(HE)TPP + CO2              | acetolactate synthase OR pyruvate dehydrogenase                                  |
| R117 | Butanoate metabolism                            | 2.2.1.6                             | ABAYE2836 OR<br>ABAYE3239 OR<br>ABAYE3240   | 2(HE)TPP + PYR -> ACLAC + THMPP            | acetolactate synthase  |
| R118 | Butanoate metabolism                            | 1.1.1.35                            | ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470   | 3HBCOA + NAD <-> AACCOA + NADH             | 3-hydroxyacyl-CoA dehydrogenase  |
| R119 | Butanoate metabolism                            | 5.1.2.3                             | ABAYE0628 OR<br>ABAYE3470   | 3HBCOA <-> R3HBCOA                         | 3-hydroxybutyryl-CoA epimerase   |
| R120 | Butanoate metabolism                            | 4.2.1.17                            | ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764 | 3HBCOA <-> CCOA                            | enoyl-CoA hydratase/isomerase OR 3-methylglutaconyl-CoA hydratase                |
| R121 | Butanoate metabolism                            | 1.1.1.-                             | ABAYE0043 OR<br>ABAYE0109 OR<br>ABAYE0479 OR<br>ABAYE1356 OR<br>ABAYE2589 OR<br>ABAYE2607 OR<br>ABAYE2613 OR<br>ABAYE2618 OR<br>ABAYE2845 OR<br>ABAYE3187 OR<br>ABAYE3378   | 1BOH + NAD <-> BUTANAL + NADH              | alcohol dehydrogenase  |
| R122 | Butanoate metabolism                            | 1.2.1.16                            | ABAYE0210 OR<br>ABAYE2329 OR<br>ABAYE2958   | SUCCSA + NAD -> SUCC + NADH                | succinate-semialdehyde dehydrogenase   |
| R123 | Butanoate metabolism                            | 1.2.1.16                            | ABAYE0210 OR<br>ABAYE2329 OR<br>ABAYE2958   | SUCCSA + NADP -> SUCC + NADPH              | succinate-semialdehyde dehydrogenase   |
| R124 | Butanoate metabolism                            | 2.6.1.19                            | ABAYE0209   | GABA + AKG <-> SUCCSA + GLU                | 4-aminobutyrate aminotransferase   |
| R125 | Butanoate metabolism                            | 4.1.3.4                             | ABAYE2292 OR<br>ABAYE2344   | 3H3MGCOA -> ACCOA + AAC                    | hydroxymethylglutaryl-CoA lyase  |
| R126 | Butanoate metabolism                            | 1.2.1.3                             | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | 3B1A + NAD -> 3BUT + NADH                  | aldehyde dehydrogenase   |
| R127 | Butanoate metabolism                            | 1.1.1.157                           | ABAYE2306 OR<br>ABAYE2368   | 3HBCOA + NADP <-> AACCOA + NADPH           | 3-hydroxybutyryl-CoA dehydrogenase   |
| R128 | Butanoate metabolism                            | 1.1.1.30                            | ABAYE1909   | 3HBUT + NAD <-> AAC + NADH                 | 3-hydroxybutyrate dehydrogenase  |
| R129 | Butanoate metabolism                            | 1.1.1.4                             | ABAYE1943   | 23BOH + NAD <-> ACT + NADH                 | (R,R)-butanediol dehydrogenase   |
| R130 | Butanoate metabolism                            | 1.1.1.5                             | ABAYE1944   | DAC + NADH -> ACT + NAD                    | acetoin dehydrogenase (DAC reductase)  |
| R131 | Butanoate metabolism                            | 1.1.1.5                             | ABAYE1944   | DAC + NADPH -> ACT + NADP                  | acetoin dehydrogenase (DAC reductase)  |
| R132 | Butanoate metabolism                            | 1.1.1.83                            | ABAYE2964   | RMAL + NAD -> PYR + CO2 + NADH             | tartrate dehydrogenase/decarboxylase OR D-malate dehydrogenase [decarboxylating] |
| R133 | Butanoate metabolism                            | 2.8.3.5                             | ABAYE1913 AND<br>ABAYE1914  | SUCCOA + AAC <-> SUCC + AACCOA             | acetoacetyl-CoA transferase  |
| R134 | Inositol metabolism                             | 1.2.1.27                            | ABAYE1296 OR<br>ABAYE3768   | 3OPP + COA + NAD -> ACCOA + CO2 + NADH     | NAD-dependent aldehyde dehydrogenase   |

| No.  | Metabolism                | EC Number            | ORF  | Reaction  | Enzyme  |
|------|---------------------------|----------------------|--|---|---|
| R135 | Oxidative phosphorylation | 1.6.5.3 AND 1.6.99.3 | (ABAYE3048 AND ABAYE3049 AND ABAYE3050 AND ABAYE3051 AND ABAYE3052 AND ABAYE3053 AND ABAYE3054 AND ABAYE3055 AND ABAYE3056 AND ABAYE3057 AND ABAYE3058 AND ABAYE3059 AND ABAYE3060) AND (ABAYE0977 OR ABAYE1736) | $\text{NADH} + \text{UQ} \rightarrow \text{NAD} + \text{UQH}_2$   | NADH dehydrogenase  |
| R136 | Oxidative phosphorylation | 1.6.5.3 AND 1.6.99.3 | (ABAYE3048 AND ABAYE3049 AND ABAYE3050 AND ABAYE3051 AND ABAYE3052 AND ABAYE3053 AND ABAYE3054 AND ABAYE3055 AND ABAYE3056 AND ABAYE3057 AND ABAYE3058 AND ABAYE3059 AND ABAYE3060) AND (ABAYE0977 OR ABAYE1736) | $\text{NADH} + \text{MK} \rightarrow \text{NAD} + \text{MKH}_2$   | NADH dehydrogenase  |
| R137 | Oxidative phosphorylation | 1.6.5.3 AND 1.6.99.3 | (ABAYE3048 AND ABAYE3049 AND ABAYE3050 AND ABAYE3051 AND ABAYE3052 AND ABAYE3053 AND ABAYE3054 AND ABAYE3055 AND ABAYE3056 AND ABAYE3057 AND ABAYE3058 AND ABAYE3059 AND ABAYE3060) AND (ABAYE0977 OR ABAYE1736) | $\text{NADH} + \text{DMK} \rightarrow \text{NAD} + \text{DMKH}_2$   | NADH dehydrogenase  |
| R138 | Oxidative phosphorylation | 1.3.99.1             | ABAYE0774 AND ABAYE0775 AND ABAYE0776 AND ABAYE0777  | $\text{FADH}_2 + \text{UQ} \rightarrow \text{FAD} + \text{UQH}_2$   | succinate dehydrogenase   |
| R139 | Oxidative phosphorylation | 2.5.1.- AND 1.10.3.- | ABAYE1385 AND ABAYE1386 AND ABAYE1387 AND ABAYE1388 AND ABAYE1389 AND ((ABAYE1636 AND ABAYE1637) OR ABAYE2219 AND ABAYE2220))  | $\text{UQH}_2 + 0.5 \text{O}_2 \rightarrow \text{UQ} + 2 \text{Hxt}$  | cytochrome complexes  |
| R140 | Oxidative phosphorylation | 3.6.1.1              | ABAYE3675  | $\text{PPI} \rightarrow 2 \text{PI}$  | inorganic diphosphatase   |
| R141 | ATP synthesis             | 3.6.3.14             | ABAYE3715 AND ABAYE3716 AND ABAYE3717 AND ABAYE3718 AND ABAYE3719 AND ABAYE3720 AND ABAYE3721 AND ABAYE3723  | $\text{ADP} + \text{PI} + 4 \text{Hxt} \leftrightarrow \text{ATP}$  | ATP synthase  |
| R142 | Oxidative phosphorylation | 2.7.4.1              | ABAYE2803  | $\text{ATP} + \text{PPI} \leftrightarrow \text{ADP} + \text{PPPI}$  | polyphosphate kinase  |
| R143 | Nitrogen metabolism       | 4.2.1.1              | ABAYE0262 OR ABAYE2809   | $\text{CO}_2 \rightarrow \text{HCO}_3$  | carbonic anhydrase  |
| R144 | Nitrogen metabolism       | 1.7.99.4             | ABAYE1546  | $\text{NO}_3 + \text{FEROC} \rightarrow \text{FERIC} + \text{NO}_2$   | nitrate reductase   |
| R145 | Nitrogen metabolism       | 1.7.1.4              | ABAYE1544  | $\text{NO}_2 + 3 \text{NADH} \rightarrow 3 \text{NAD} + \text{NH}_3$  | nitrite reductase   |
| R146 | Nitrogen metabolism       | 1.7.1.4              | ABAYE1544  | $\text{NO}_2 + 3 \text{NADPH} \rightarrow 3 \text{NADP} + \text{NH}_3$  | nitrite reductase   |
| R147 | Nitrogen metabolism       | 4.3.1.1              | ABAYE1921  | $\text{ASP} \leftrightarrow \text{FUM} + \text{NH}_3$   | aspartate ammonia-lyase   |
| R148 | Nitrogen metabolism       | 1.13.11.32           | ABAYE0966 OR ABAYE2310   | $\text{O}_2 + 2 \text{2NPRPN} \leftrightarrow 2 \text{ACTN} + 2 \text{NO}_2$                                      | 2-nitropropane dioxygenase  |
| R149 | Nitrogen metabolism       | 1.14.12.1            | ABAYE1896 AND ABAYE1897  | $\text{AN} + \text{O}_2 + \text{NADH} \leftrightarrow \text{CATECHOL} + \text{NH}_3 + \text{CO}_2 + \text{NAD}$   | anthranilate dioxygenase  |
| R150 | Nitrogen metabolism       | 1.14.12.1            | ABAYE1896 AND ABAYE1897  | $\text{AN} + \text{O}_2 + \text{NADPH} \leftrightarrow \text{CATECHOL} + \text{NH}_3 + \text{CO}_2 + \text{NADP}$ | anthranilate dioxygenase  |
| R151 | Nitrogen metabolism       | 1.4.1.13             | ABAYE0298 AND ABAYE0299  | $2 \text{GLU} + \text{NADP} \leftrightarrow \text{GLN} + \text{AKG} + \text{NADPH}$                               | glutamate synthase  |
| R152 | Nitrogen metabolism       | 1.4.1.13             | ABAYE0298 AND ABAYE0299  | $2 \text{GLU} + \text{NAD} \leftrightarrow \text{GLN} + \text{AKG} + \text{NADH}$                                 | glutamate synthase  |
| R153 | Nitrogen metabolism       | 1.4.1.3 OR 1.4.1.4   | ABAYE0351 OR ABAYE2764   | $\text{GLU} + \text{NAD} \leftrightarrow \text{AKG} + \text{NH}_3 + \text{NADH}$                                  | glutamate dehydrogenase (NAD(P)+) oxidoreductase protein                |
| R154 | Nitrogen metabolism       | 1.4.1.3 OR 1.4.1.4   | ABAYE0351 OR ABAYE2764   | $\text{GLU} + \text{NADP} \leftrightarrow \text{AKG} + \text{NH}_3 + \text{NADPH}$                                | glutamate dehydrogenase, NADP-specific                                  |
| R155 | Nitrogen metabolism       | 1.4.99.1             | ABAYE1567 OR ABAYE3774   | $\text{DALA} + \text{FAD} \leftrightarrow \text{PYR} + \text{NH}_3 + \text{FADH}_2$                               | D-amino acid dehydrogenase  |
| R156 | Sulfur metabolism         | 2.7.7.4              | ABAYE2790 AND ABAYE2791  | $\text{SLF} + \text{ATP} \rightarrow \text{PPI} + \text{APS}$   | sulfate adenyltransferase   |
| R157 | Sulfur metabolism         | 2.7.1.25             |  | $\text{APS} + \text{ATP} \rightarrow \text{ADP} + \text{PAPS}$  | adenylylsulfate kinase  |
| R158 | Sulfur metabolism         | 1.8.4.8              | ABAYE0709  | $\text{PAPS} + \text{RTHIO} \rightarrow \text{OTHIO} + \text{H}_2\text{SO}_3 + \text{PAP}$                        | 3'-phosphoadenosine 5'-phosphosulfate sulfotransferase (PAPS reductase) |
| R159 | Sulfur metabolism         | 1.8.1.2              | ABAYE0634 OR ABAYE0682   | $\text{H}_2\text{SO}_3 + 3 \text{NADPH} \rightarrow \text{H}_2\text{S} + 3 \text{NADP}$                           | sulfite reductase (NADPH)   |
| R160 | Sulfur metabolism         | 3.1.3.7              |  | $\text{PAP} \rightarrow \text{PI} + \text{AMP}$   | 3',5'-bisphosphate nucleotidase   |
| R161 | Sulfur metabolism         | 1.8.1.2              | ABAYE0634  | $\text{SELT} + 3 \text{NADP} \rightarrow \text{SELD} + 3 \text{NADPH}$  | sulfite reductase (NADPH)   |

| No.  | Metabolism   | EC Number  | ORF   | Reaction   | Enzyme  |
|------|--|--|---|--|---|
| R162 | Fatty acid biosynthesis                                | 6.4.1.2 AND<br>6.3.4.14  | (ABAYE0614 OR<br>ABAYE1537 OR<br>ABAYE1538 OR<br>ABAYE3153) AND<br>(ABAYE1537 OR<br>ABAYE2291 OR<br>ABAYE2438)                  | ACCOA + ATP + HCO <sub>3</sub> -> MALCOA + ADP + PI                              | acetyl-CoA carboxylase                            |
| R163 | Fatty acid biosynthesis                                | 2.3.1.39   | ABAYE2227 OR<br>ABAYE2993   | MALCOA + ACP -> MALACP + COA   | malonyl CoA-acyl carrier protein transacylase     |
| R164 | Fatty acid biosynthesis                                | 2.3.1.180  | ABAYE2562   | ACCOA + ACP -> ACACP + COA   | 3-oxoacyl-[acyl-carrier-protein] synthase         |
| R165 | Fatty acid biosynthesis                                |  |   | PPACOA + ACP -> PPAACP + COA   | malonyl CoA-acyl carrier protein transacylase     |
| R166 | Fatty acid biosynthesis<br>(nonanoic acid; c9:0)       | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | PPAACP + 3 MALACP + 6 NADPH -> 6 NADP +<br>C090ACP + 3 CO <sub>2</sub> + 3 ACP   | synthesis of nonanoyl-[acyl-carrier protein]      |
| R167 | Fatty acid biosynthesis<br>(decanoic acid; c10:0)      | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | ACACP + 4 MALACP + 8 NADPH -> 8 NADP +<br>C100ACP + 4 CO <sub>2</sub> + 4 ACP    | synthesis of decanoyl-[acyl-carrier protein]      |
| R168 | Fatty acid biosynthesis<br>(undecanoic acid; c11:0)    | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | PPAACP + 4 MALACP + 8 NADPH -> 8 NADP +<br>C110ACP + 4 CO <sub>2</sub> + 4 ACP   | synthesis of undecanoyl-[acyl-carrier protein]    |
| R169 | Fatty acid biosynthesis<br>(dodecanoic acid; c12:0)    | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | ACACP + 5 MALACP + 10 NADPH -> 10 NADP +<br>C120ACP + 5 CO <sub>2</sub> + 5 ACP  | synthesis of dodecanoyl-[acyl-carrier protein]    |
| R170 | Fatty acid biosynthesis<br>(tridecanoic acid; c13:0)   | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | PPAACP + 5 MALACP + 10 NADPH -> 10 NADP +<br>C130ACP + 5 CO <sub>2</sub> + 5 ACP | synthesis of tridecanoyl-[acyl-carrier protein]   |
| R171 | Fatty acid biosynthesis<br>(tetradecanoic acid; c14:0) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | ACACP + 6 MALACP + 12 NADPH -> 12 NADP +<br>C140ACP + 6 CO <sub>2</sub> + 6 ACP  | synthesis of tetradecanoyl-[acyl-carrier protein] |
| R172 | Fatty acid biosynthesis<br>(pentadecanoic acid; c15:0) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | PPAACP + 6 MALACP + 12 NADPH -> 12 NADP +<br>C150ACP + 6 CO <sub>2</sub> + 6 ACP | synthesis of pentadecanoyl-[acyl-carrier protein] |
| R173 | Fatty acid biosynthesis<br>(pentadecenoic acid; c15:1) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | PPAACP + 6 MALACP + 11 NADPH -> 11 NADP +<br>C151ACP + 6 CO <sub>2</sub> + 6 ACP | synthesis of pentadecenoyl-[acyl-carrier protein] |
| R174 | Fatty acid biosynthesis<br>(hexadecanoic acid; c16:0)  | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | ACACP + 7 MALACP + 14 NADPH -> 14 NADP +<br>C160ACP + 7 CO <sub>2</sub> + 7 ACP  | synthesis of hexadecanoyl-[acyl-carrier protein]  |
| R175 | Fatty acid biosynthesis<br>(hexadecenoic acid; c16:1)  | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | ACACP + 7 MALACP + 13 NADPH -> 13 NADP +<br>C161ACP + 7 CO <sub>2</sub> + 7 ACP  | synthesis of hexadecenoyl-[acyl-carrier protein]  |
| R176 | Fatty acid biosynthesis<br>(heptadecanoic acid; c17:0) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | PPAACP + 7 MALACP + 14 NADPH -> 14 NADP +<br>C170ACP + 7 CO <sub>2</sub> + 7 ACP | synthesis of heptadecanoyl-[acyl-carrier protein] |
| R177 | Fatty acid biosynthesis<br>(heptadecenoic acid; c17:1) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.- | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586 | PPAACP + 7 MALACP + 13 NADPH -> 13 NADP +<br>C171ACP + 7 CO <sub>2</sub> + 7 ACP | synthesis of heptadecenoyl-[acyl-carrier protein] |

| No.  | Metabolism  | EC Number   | ORF   | Reaction  | Enzyme   |
|------|---|---|---|---|--|
| R178 | Fatty acid biosynthesis<br>(octadecanoic acid; c18:0) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.-  | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586   | ACACP + 8 MALACP + 16 NADPH -> 16 NADP +<br>C180ACP + 8 CO2 + 8 ACP             | synthesis of octadecanoyl-[acyl-carrier protein] |
| R179 | Fatty acid biosynthesis<br>(octadecenoic acid; c18:1) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.-  | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586   | ACACP + 8 MALACP + 15 NADPH -> 15 NADP +<br>C181ACP + 8 CO2 + 8 ACP             | synthesis of octadecenoyl-[acyl-carrier protein] |
| R180 | Fatty acid biosynthesis<br>(nonadecanoic acid; c19:0) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.-  | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586   | PPAACP + 8 MALACP + 16 NADPH -> 16 NADP +<br>C190ACP + 8 CO2 + 8 ACP            | synthesis of nonadecanoyl-[acyl-carrier protein] |
| R181 | Fatty acid biosynthesis<br>(nonadecenoic acid; c19:1) | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.-  | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586   | PPAACP + 8 MALACP + 15 NADPH -> 15 NADP +<br>C191ACP + 8 CO2 + 8 ACP            | synthesis of nonadecenoyl-[acyl-carrier protein] |
| R182 | Fatty acid biosynthesis<br>(eicosanoic acid; c20:0)   | 1.1.1.100 AND<br>1.3.1.9 AND<br>2.3.1.41 AND<br>2.3.1.180 AND<br>4.2.1.-  | (ABAYE1514 OR<br>ABAYE1706 OR<br>ABAYE2246 OR<br>ABAYE2992) AND<br>ABAYE3250 AND<br>ABAYE2951 AND<br>ABAYE2562 AND<br>ABAYE1586   | ACACP + 9 MALACP + 18 NADPH -> 18 NADP +<br>C200ACP + 9 CO2 + 9 ACP             | synthesis of eicosanoyl-[acyl-carrier protein]   |
| R183 | Fatty acid metabolism<br>(decanoic acid; c10:0)       | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C100 + 5 COA + 4 FAD + 4 NAD + ATP -> 5 ACCOA<br>+ 4 FADH2 + 4 NADH + AMP + PPI | oxidation of decanoic acid                       |
| R184 | Fatty acid metabolism<br>(dodecanoic acid; c12:0)     | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C120 + 6 COA + 5 FAD + 5 NAD + ATP -> 6 ACCOA<br>+ 5 FADH2 + 5 NADH + AMP + PPI | oxidation of dodecanoic acid                     |

| No.  | Metabolism   | EC Number   | ORF   | Reaction   | Enzyme                          |
|------|--|---|---|--|---------------------------------|
| R185 | Fatty acid metabolism<br>(tetradecanoic acid; c14:0) | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C140 + 7 COA + 6 FAD + 6 NAD + ATP -> 7 ACCOA<br>+ 6 FADH2 + 6 NADH + AMP + PPI          | oxidation of tetradecanoic acid |
| R186 | Fatty acid metabolism<br>(pentadecanoic acid; c15:0) | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C150 + 7 COA + 6 FAD + 6 NAD + ATP -> 6 ACCOA<br>+ PPACOA + 6 FADH2 + 6 NADH + AMP + PPI | oxidation of pentadecanoic acid |
| R187 | Fatty acid metabolism<br>(hexadecanoic acid; c16:0)  | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C160 + 8 COA + 7 FAD + 7 NAD + ATP -> 8 ACCOA<br>+ 7 FADH2 + 7 NADH + AMP + PPI          | oxidation of hexadecanoic acid  |
| R188 | Fatty acid metabolism<br>(hexadecenoic acid; c16:1)  | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C161 + 8 COA + 7 FAD + 7 NAD + ATP -> 8 ACCOA<br>+ 7 FADH2 + 7 NADH + AMP + PPI          | oxidation of hexadecenoic acid  |



| No.  | Metabolism   | EC Number   | ORF   | Reaction   | Enzyme                          |
|------|--|---|---|--|---------------------------------|
| R189 | Fatty acid metabolism<br>(heptadecanoic acid; c17:0) | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C170 + 8 COA + 7 FAD + 7 NAD + ATP -> 7 ACCOA<br>+ PPACOA + 7 FADH2 + 7 NADH + AMP + PPI | oxidation of heptadecanoic acid |
| R190 | Fatty acid metabolism<br>(heptadecenoic acid; c17:1) | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C171 + 8 COA + 7 FAD + 7 NAD + ATP -> 7 ACCOA<br>+ PPACOA + 7 FADH2 + 7 NADH + AMP + PPI | oxidation of heptadecenoic acid |
| R191 | Fatty acid metabolism<br>(octadecanoic acid; c18:0)  | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C180 + 9 COA + 8 FAD + 8 NAD + ATP -> 9 ACCOA<br>+ 8 FADH2 + 8 NADH + AMP + PPI          | oxidation of octadecanoic acid  |
| R192 | Fatty acid metabolism<br>(octadecenoic acid; c18:1)  | 6.2.1.3 AND<br>1.3.99.- AND<br>1.3.99.3 AND<br>1.3.99.13 AND<br>4.2.1.17 AND<br>1.1.1.35 AND<br>2.3.1.16 AND<br>2.3.1.9 AND<br>1.3.99.7 | (ABAYE2630 OR<br>ABAYE3678) AND<br>ABAYE1145 AND<br>(ABAYE0436 OR<br>ABAYE1204 OR<br>ABAYE2631) AND<br>(ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470) AND<br>(ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3470 OR<br>ABAYE3763 OR<br>ABAYE3764) AND<br>ABAYE3097 AND<br>ABAYE3471 | C181 + 9 COA + 8 FAD + 8 NAD + ATP -> 9 ACCOA<br>+ 8 FADH2 + 8 NADH + AMP + PPI          | oxidation of octadecenoic acid  |
| R193 | Fatty acid metabolism                                | 1.14.15.3   | ABAYE2014   | C120ACP + O2 + RRBRDX <-> C120OH +<br>ORBRDX + ACP                                       | terminal alkane-1-monooxygenase |
| R194 | Fatty acid metabolism                                | 1.14.15.3   | ABAYE2014   | C120ACP + O2 + FADH2 <-> C120OH + FAD +<br>ACP   | terminal alkane-1-monooxygenase |

| No.  | Metabolism                     | EC Number               | ORF   | Reaction   | Enzyme  |
|------|--------------------------------|-------------------------|---|--|---|
| R195 | Fatty acid metabolism          | 1.14.15.3               | ABAYE2014   | C140ACP + O2 + RRBRDX <=> C140OH + ORBRDX + ACP  | terminal alkane-1-monoxygenase  |
| R196 | Fatty acid metabolism          | 1.14.15.3               | ABAYE2014   | C140ACP + O2 + FADH2 <=> C140OH + FAD + ACP  | terminal alkane-1-monoxygenase  |
| R197 | Fatty acid metabolism          | 1.1.1.1                 | ABAYE0763 OR<br>ABAYE1463 OR<br>ABAYE1522 OR<br>ABAYE1861 OR<br>p2ABAYE0004 OR<br>p3ABAYE0020 OR<br>p3ABAYE0024   | CH3OR + NAD <=> RCHO + NADH  | alcohol dehydrogenase   |
| R198 | Fatty acid metabolism          | 1.14.15.3               | ABAYE2014   | RH + RRBRDX + O2 <=> ORBRDX + CH3OR  | terminal alkane-1-monoxygenase  |
| R199 | Fatty acid metabolism          | 1.18.1.1 OR<br>1.18.1.3 | (ABAYE1067 OR<br>ABAYE2799) OR<br>ABAYE2843   | RRBRDX + NAD <=> ORBRDX + NADH   | rubredoxin-NAD(+) reductase OR ferredoxin reductase component (dioxxygenase)        |
| R200 | Fatty acid metabolism          | 1.18.1.3                | ABAYE2843   | RRBRDX + NADP <=> ORBRDX + NADPH   | ferredoxin reductase component (dioxxygenase)                                       |
| R201 | Fatty acid metabolism          | 1.2.1.3                 | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | RCHO + NAD <=> 0.015 C100 + 0.048 C120 + 0.003 C140 + 0.003 C150 + 0.281 C160 + 0.192 C161 + 0.017 C170 + 0.016 C171 + 0.008 C180 + 0.375 C181 + 0.041 C120OH + NADH                                     | aldehyde dehydrogenase  |
| R202 | Fatty acid metabolism          | 5.3.3.8                 | ABAYE3470   | C121COA <=> C122COA  | fatty oxidation complex alpha subunit   |
| R203 | Biosynthesis of steroids       | 2.2.1.7                 | ABAYE0381   | PYR + G3P -> DX5P + CO2  | 1-deoxy-D-xylulose-5-phosphate synthase   |
| R204 | Biosynthesis of steroids       | 1.1.1.267               | ABAYE1581   | DX5P + NADPH -> MDE4P + NADP   | 1-deoxy-D-xylulose-5-phosphate reductoisomerase                                     |
| R205 | Biosynthesis of steroids       | 2.7.7.60                | ABAYE1672   | MDE4P + CTP -> CDPMDE + PPI  | 4-diphosphocytidyl-2-methyl-D-erythritol synthase                                   |
| R206 | Biosynthesis of steroids       | 4.6.1.12                | ABAYE1569   | 2PCDPMDE -> MDECPP + CMP   | 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase                               |
| R207 | Biosynthesis of steroids       | 1.17.4.3                | ABAYE3263   | MDECPP + NADH -> NAD + HMB4PP  | 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase                                |
| R208 | Biosynthesis of steroids       | 1.17.1.2                | ABAYE0313   | HMB4PP + NADH -> NAD + IPP   | 4-hydroxy-3-methylbut-2-enyl diphosphate reductase                                  |
| R209 | Biosynthesis of steroids       | 2.5.1.10                | ABAYE0722   | DMPP + IPP -> GPP + PPI  | geranylgeranyl pyrophosphate synthase   |
| R210 | Biosynthesis of steroids       | 2.5.1.10                | ABAYE0722   | GPP + IPP -> FPP + PPI   | geranylgeranyl pyrophosphate synthase   |
| R211 | Biosynthesis of steroids       |                         |   | GGPP + IPP -> PPPP + PPI   | dimethylallyltransferase  |
| R212 | Biosynthesis of steroids       |                         |   | HEPPP + IPP -> OPP + PPI   | trans-hexaprenyltransferase   |
| R213 | Glycerolipid metabolism        | 2.7.1.31                | ABAYE0849   | 3PG + ADP <=> DGLYCERATE + ATP   | glycerate kinase  |
| R214 | Glycerolipid metabolism        | 1.2.1.3                 | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | NADH + DGLYCERATE <=> T3 + NAD   | aldehyde dehydrogenase  |
| R215 | Glycerolipid metabolism        | 2.7.1.30                | ABAYE0816   | GL + ATP -> GL3P + ADP   | glycerol kinase   |
| R216 | Glycerolipid metabolism        | 3.1.1.3                 | ABAYE0325 OR<br>ABAYE2810   | DGR -> AGL + 0.015 C100 + 0.048 C120 + 0.003 C140 + 0.003 C150 + 0.281 C160 + 0.192 C161 + 0.017 C170 + 0.016 C171 + 0.008 C180 + 0.375 C181 + 0.041 C120OH  | triacylglycerol lipase  |
| R217 | Glycerolipid metabolism        | 3.1.1.3                 | ABAYE0325 OR<br>ABAYE2810   | TGL -> DGR + 0.015 C100 + 0.048 C120 + 0.003 C140 + 0.003 C150 + 0.281 C160 + 0.192 C161 + 0.017 C170 + 0.016 C171 + 0.008 C180 + 0.375 C181 + 0.041 C120OH  | triacylglycerol lipase  |
| R218 | Glycerolipid metabolism        | 2.3.1.15                | ABAYE0397   | GL3P + ACCOA -> AGL3P + COA  | glycerol-3-phosphate acyltransferase  |
| R219 | Glycerolipid metabolism        | 2.3.1.20                | ABAYE0708   | TGL + COA -> DGR + 0.015 C100 + 0.048 C120 + 0.003 C140 + 0.003 C150 + 0.281 C160 + 0.192 C161 + 0.017 C170 + 0.016 C171 + 0.008 C180 + 0.375 C181 + 0.041 C120OH  | bifunctional protein [wax ester synthase / acyl-CoA:diacylglycerol acyltransferase] |
| R220 | Glycerophospholipid metabolism | 1.1.1.94                | ABAYE1223   | DHAP + NADH -> GL3P + NAD  | glycerol-3-phosphate dehydrogenase  |
| R221 | Glycerophospholipid metabolism | 1.1.1.94                | ABAYE1223   | DHAP + NADPH -> GL3P + NADP  | glycerol-3-phosphate dehydrogenase  |
| R222 | Glycerophospholipid metabolism | 1.1.99.5                | ABAYE0817   | DHAP + UQH2 <=> GL3P + UQ  | glycerol-3-phosphate dehydrogenase  |
| R223 | Glycerophospholipid metabolism | 1.1.99.5                | ABAYE0817   | DHAP + MKH2 <=> GL3P + MK  | glycerol-3-phosphate dehydrogenase  |
| R224 | Glycerophospholipid metabolism | 1.1.99.5                | ABAYE0817   | DHAP + DMKH2 <=> GL3P + DMK  | glycerol-3-phosphate dehydrogenase  |
| R225 | Glycerophospholipid metabolism | 2.3.1.-                 | ABAYE0497 OR<br>ABAYE0625 OR<br>ABAYE1513 OR<br>ABAYE1675 OR<br>ABAYE1715 OR<br>ABAYE1811 OR<br>ABAYE2153 OR<br>ABAYE2367 OR<br>ABAYE2457 OR<br>ABAYE2483 OR<br>ABAYE3572 OR<br>ABAYE3588 OR<br>ABAYE3697 OR<br>ABAYE3807 | GL3P + ACCOA -> 2AGL3P + COA   | acetyltransferase   |
| R226 | Glycerophospholipid metabolism | 2.3.1.15                | ABAYE0397   | GL3P + 0.015 C100ACP + 0.048 C120ACP + 0.003 C140ACP + 0.003 C150ACP + 0.281 C160ACP + 0.192 C161ACP + 0.017 C170ACP + 0.016 C171ACP + 0.008 C180ACP + 0.375 C181ACP + 0.041 C120OH -> AGL3P + 0.958 ACP | glycerol-3-phosphate O-acyltransferase  |
| R227 | Glycerophospholipid metabolism | 2.3.1.51                |   | AGL3P + 0.015 C100ACP + 0.048 C120ACP + 0.003 C140ACP + 0.003 C150ACP + 0.281 C160ACP + 0.192 C161ACP + 0.017 C170ACP + 0.016 C171ACP + 0.008 C180ACP + 0.375 C181ACP + 0.041 C120OH -> PA + 0.958 ACP   | 1-acylglycerol-3-phosphate O-acyltransferase  |
| R228 | Glycerophospholipid metabolism | 2.7.1.107               | ABAYE0824   | DGR + ATP -> ADP + PA  | diacylglycerol kinase   |
| R229 | Glycerophospholipid metabolism | 3.1.1.32                | ABAYE1646   | PC -> 2AG3PC + 0.015 C100 + 0.048 C120 + 0.003 C140 + 0.003 C150 + 0.281 C160 + 0.192 C161 + 0.017 C170 + 0.016 C171 + 0.008 C180 + 0.375 C181 + 0.041 C120OH  | phospholipase   |
| R230 | Glycerophospholipid metabolism | 3.1.4.46                | ABAYE0604 OR<br>ABAYE0826   | G3PC -> CHOLINE + GL3P   | glycerophosphoryl diester phosphodiesterase   |
| R231 | Glycerophospholipid metabolism | 2.7.7.41                | ABAYE1580   | PA + CTP <=> CDPDG + PPI   | phosphatidate cytidyltransferase  |
| R232 | Glycerophospholipid metabolism | 2.7.8.8                 | ABAYE0470   | CDPDG + SER <=> CMP + PS   | phosphatidylserine synthase   |
| R233 | Glycerophospholipid metabolism | 3.1.1.32                | ABAYE1646   | PS -> 2AG3PS + 0.015 C100 + 0.048 C120 + 0.003 C140 + 0.003 C150 + 0.281 C160 + 0.192 C161 + 0.017 C170 + 0.016 C171 + 0.008 C180 + 0.375 C181 + 0.041 C120OH  | phospholipase   |
| R234 | Glycerophospholipid metabolism | 4.1.1.65                | ABAYE0104   | PS -> PE + CO2   | phosphatidylserine decarboxylase  |
| R235 | Glycerophospholipid metabolism | 3.1.1.32                | ABAYE1646   | PE -> 2AG3PE + 0.015 C100 + 0.048 C120 + 0.003 C140 + 0.003 C150 + 0.281 C160 + 0.192 C161 + 0.017 C170 + 0.016 C171 + 0.008 C180 + 0.375 C181 + 0.041 C120OH  | phospholipase   |
| R236 | Glycerophospholipid metabolism | 3.1.4.46                | ABAYE0604 OR<br>ABAYE0826   | G3PE -> ETHA + GL3P  | glycerophosphoryl diester phosphodiesterase   |

| No.  | Metabolism                      | EC Number | ORF                                 | Reaction                                  | Enzyme  |
|------|---------------------------------|-----------|-------------------------------------|---|---|
| R237 | Glycerophospholipid metabolism  | 2.7.8.5   | ABAYE3463                           | CDPDG + GL3P <=> CMP + PGP                | CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase   |
| R238 | Glycerophospholipid metabolism  | 3.1.3.27  | ABAYE0091 OR ABAYE0749 OR ABAYE3269 | PGP -> PI + PG                            | phosphatidylglycerophosphatase  |
| R239 | Glycerophospholipid metabolism  | 2.7.8.-   |                                     | CDPDG + PG -> CMP + CL                    | cardiolipin synthase  |
| R240 | Glycerophospholipid metabolism  | 3.1.4.3   | ABAYE1520 OR ABAYE3825              | PC <=> DGR + CHOLINEP                     | phospholipase C precursor (phosphatidylcholine cholinephosphohydrolase) (phosphatidylcholine-hydrolyzing phospholipase C) |
| R241 | Glycerophospholipid metabolism  | 3.1.4.3   | ABAYE1520 OR ABAYE3825              | PE <=> DGR + ETHAP                        | phospholipase C precursor (phosphatidylcholine cholinephosphohydrolase) (phosphatidylcholine-hydrolyzing phospholipase C) |
| R242 | Glycerophospholipid metabolism  | 3.1.4.3   | ABAYE1520 OR ABAYE3825              | PG <=> DGR + GL3P                         | phospholipase C precursor (phosphatidylcholine cholinephosphohydrolase) (phosphatidylcholine-hydrolyzing phospholipase C) |
| R243 | Glycerophospholipid metabolism  | 4.3.1.7   | ABAYE1457 AND ABAYE1458             | ETHA <=> ACAL + NH3                       | ethanolamine ammonia-lyase  |
| R244 | Purine metabolism               | 2.7.6.1   | ABAYE1789 OR ABAYE2981              | R5P + ATP <=> PRPP + AMP                  | ribose-phosphate pyrophosphokinase  |
| R245 | Purine metabolism (De novo)     | 2.4.2.14  | ABAYE1280                           | PRPP + GLN -> PRAM + PPI + GLU            | amidophosphoribosyltransferase  |
| R246 | Purine metabolism (De novo)     | 6.3.4.13  | ABAYE1366                           | PRAM + ATP + GLY <=> GAR + ADP + PI       | phosphoribosylamine-glycine ligase  |
| R247 | Purine metabolism (De novo)     | 2.1.2.2   | ABAYE0888 OR ABAYE2179              | GAR + FTHF -> FGAR + THF                  | phosphoribosylglycinamide formyltransferase   |
| R248 | Purine metabolism (De novo)     | 6.3.5.3   | ABAYE0912                           | FGAR + ATP + GLN -> FGAM + GLU + ADP + PI | phosphoribosylformylglycinamide synthase  |
| R249 | Purine metabolism (De novo)     | 6.3.3.1   | ABAYE0889                           | FGAM + ATP -> AIR + ADP + PI              | phosphoribosylformylglycinamide cyclo-lyase   |
| R250 | Purine metabolism (De novo)     | 4.1.1.21  | ABAYE3871 AND ABAYE3872             | AIR + CO2 + ATP -> CAIR + ADP + PI        | phosphoribosylaminoimidazole carboxylase  |
| R251 | Purine metabolism (De novo)     | 6.3.2.6   | ABAYE0056                           | CAIR + ATP + ASP <=> SAICAR + ADP + PI    | phosphoribosylaminoimidazole-succinocarboxamide synthase  |
| R252 | Purine metabolism (De novo)     | 4.3.2.2   | ABAYE1039                           | SAICAR <=> AICAR + FUM                    | adenylosuccinate lyase  |
| R253 | Purine metabolism (De novo)     | 2.1.2.3   | ABAYE1367                           | AICAR + FTHF <=> PRFICA + THF             | phosphoribosylaminoimidazolecarboxamide formyltransferase   |
| R254 | Purine metabolism (De novo)     | 3.5.4.10  | ABAYE1367                           | PRFICA <=> IMP                            | phosphoribosylaminoimidazolecarboxamide formyltransferase; IMP cyclohydrolase   |
| R255 | Purine metabolism (De novo)     | 6.3.4.4   | ABAYE2592                           | IMP + GTP + ASP -> ASUC + GDP + PI        | adenylosuccinate synthase   |
| R256 | Purine metabolism (De novo)     | 4.3.2.2   | ABAYE1039                           | ASUC <=> FUM + AMP                        | adenylosuccinate lyase  |
| R257 | Purine metabolism (De novo)     | 1.1.1.205 | ABAYE0166                           | IMP + NAD -> XMP + NADH                   | IMP dehydrogenase   |
| R258 | Purine metabolism (De novo)     | 6.3.5.2   | ABAYE1456 OR ABAYE3740              | XMP + ATP + GLN -> GMP + GLU + AMP + PPI  | GMP synthetase  |
| R259 | Purine metabolism               | 3.5.4.4   | ABAYE2601 OR ABAYE3101              | ADN -> INS + NH3                          | adenosine deaminase   |
| R260 | Purine metabolism               | 3.5.4.4   | ABAYE2601 OR ABAYE3101              | DA <=> DIN + NH3                          | adenosine deaminase   |
| R261 | Purine metabolism               | 3.1.3.5   | ABAYE1047 OR ABAYE1886              | IMP -> INS + PI                           | 5'-nucleotidase   |
| R262 | Purine metabolism               | 3.1.3.5   | ABAYE1047 OR ABAYE1886              | AMP -> ADN + PI                           | 5'-nucleotidase   |
| R263 | Purine metabolism               | 3.1.3.5   | ABAYE1047 OR ABAYE1886              | XMP -> XTSINE + PI                        | 5'-nucleotidase   |
| R264 | Purine metabolism               | 3.1.3.5   | ABAYE1047 OR ABAYE1886              | GMP -> GSN + PI                           | 5'-nucleotidase   |
| R265 | Purine metabolism               | 3.1.3.5   | ABAYE1047 OR ABAYE1886              | DAMP <=> DA + PI                          | 5'-nucleotidase   |
| R266 | Purine metabolism               | 3.1.3.5   | ABAYE1047 OR ABAYE1886              | DGMP <=> DG + PI                          | 5'-nucleotidase   |
| R267 | Purine metabolism               | 2.7.4.8   | ABAYE0312                           | DGMP + ATP <=> DGDP + ADP                 | guanylate kinase  |
| R268 | Purine metabolism               | 2.7.4.6   | ABAYE3267                           | IDP + ATP <=> ITP + ADP                   | nucleoside-diphosphate kinase   |
| R269 | Purine metabolism               | 2.7.4.6   | ABAYE3267                           | ATP + DIDP <=> ADP + DITP                 | nucleoside-diphosphate kinase   |
| R270 | Purine metabolism               | 2.4.2.8   | ABAYE3887                           | HYXN + PRPP -> PPI + IMP                  | hypoxanthine phosphoribosyltransferase  |
| R271 | Purine metabolism               | 2.4.2.8   | ABAYE3887                           | XAN + PRPP -> PPI + XMP                   | hypoxanthine phosphoribosyltransferase  |
| R272 | Purine metabolism               | 2.4.2.8   | ABAYE3887                           | AMP + PPI <=> AD + PRPP                   | hypoxanthine phosphoribosyltransferase  |
| R273 | Purine metabolism               | 3.1.5.1   | ABAYE0911                           | DGTP -> DG + PPPI                         | dGTP triphosphohydrolase  |
| R274 | Purine metabolism               | 2.7.6.5   | ABAYE3181                           | ATP + GTP -> pppGpp + AMP                 | GTP pyrophosphokinase   |
| R275 | Purine metabolism               | 3.1.7.2   | ABAYE0310                           | ppGpp <=> GDP + PPI                       | guanosine-3',5'-bis(diphosphate) 3'-pyrophosphohydrolase  |
| R276 | Purine metabolism               | 2.7.4.3   | ABAYE2767                           | ATP + AMP <=> 2 ADP                       | adenylylate kinase  |
| R277 | Purine metabolism               | 1.17.4.1  | ABAYE3065 AND ABAYE3067             | ADP + RTHIO -> DADP + OTHIO               | ribonucleoside-diphosphate reductase  |
| R278 | Purine metabolism               | 2.7.4.6   | ABAYE3267                           | DADP + ATP <=> DATP + ADP                 | nucleoside-diphosphate kinase   |
| R279 | Purine metabolism               | 2.7.4.8   | ABAYE0312                           | GMP + ATP <=> GDP + ADP                   | guanylate kinase  |
| R280 | Purine metabolism               | 2.7.4.6   | ABAYE3267                           | GDP + ATP <=> GTP + ADP                   | nucleoside-diphosphate kinase   |
| R281 | Purine metabolism               | 1.17.4.1  | ABAYE3065 AND ABAYE3067             | GDP + RTHIO -> DGDP + OTHIO               | ribonucleoside-diphosphate reductase  |
| R282 | Purine metabolism               | 2.7.4.6   | ABAYE3267                           | DGDP + ATP <=> DGTP + ADP                 | nucleoside-diphosphate kinase   |
| R283 | Purine metabolism               | 3.6.1.13  | ABAYE3519                           | ARIB -> AMP + R5P                         | ADPribose ribophosphohydrolase  |
| R284 | Purine metabolism               | 2.7.4.3   | ABAYE2767                           | ATP + DAMP <=> ADP + DADP                 | adenylylate kinase  |
| R285 | Purine metabolism               | 3.6.1.41  | ABAYE0491                           | AppppA -> 2 ADP                           | bis(5'-nucleosyl)-tetrphosphatase   |
| R286 | Purine metabolism               | 1.17.1.4  | ABAYE1114 AND ABAYE1115             | HYXN + NAD <=> XAN + NADH                 | xanthine dehydrogenase  |
| R287 | Purine metabolism               | 1.17.1.4  | ABAYE1114 AND ABAYE1115             | XAN + NAD <=> URT + NADH                  | xanthine dehydrogenase  |
| R288 | Purine metabolism               | 3.5.3.19  | ABAYE0127                           | UDGLYCOLATE <=> GLX + 2 NH3 + CO2         | ureidoglycolate amidohydrolase(decarboxylating)   |
| R289 | Purine metabolism               | 3.5.3.4   | ABAYE0128                           | ALLNT <=> UDGLYCOLATE + UREA              | allantoicase  |
| R290 | Purine metabolism               | 3.5.4.3   | ABAYE2396 OR ABAYE3885              | GN <=> XAN + NH3                          | guanine deaminase   |
| R291 | Purine metabolism               | 3.6.1.11  | ABAYE3154                           | pppGpp -> ppGpp + PI                      | exopolyphosphatase (exopolypase)  |
| R292 | Purine metabolism               | 3.6.1.15  | ABAYE3296                           | ATP <=> ADP + PI                          | hypothetical protein  |
| R293 | Purine metabolism               | 3.6.1.19  | ABAYE3179                           | DITP -> DIMP + PPI                        | nucleoside-triphosphate pyrophosphatase   |
| R294 | Purine metabolism               | 3.6.1.19  | ABAYE3179                           | GTP -> GMP + PPI                          | nucleoside-triphosphate pyrophosphatase   |
| R295 | Purine metabolism               | 3.6.1.19  | ABAYE3179                           | ITP -> IMP + PPI                          | nucleoside-triphosphate pyrophosphatase   |
| R296 | Purine metabolism               | 3.6.1.19  | ABAYE3179                           | XTP -> XMP + PPI                          | nucleoside-triphosphate pyrophosphatase   |
| R297 | Purine metabolism               | 3.6.1.19  | ABAYE3179                           | DGTP -> DGMP + PPI                        | nucleoside-triphosphate pyrophosphatase   |
| R298 | Purine metabolism               | 4.1.1.-   | ABAYE1027                           | 5AI + CO2 <=> 5A4ICA                      | L-2,4-diaminobutyrate decarboxylase   |
| R299 | Pyrimidine metabolism (De novo) | 2.1.3.2   | ABAYE2578                           | CAP + ASP -> CAASP + PI                   | aspartate carbamoyltransferase  |
| R300 | Pyrimidine metabolism (De novo) | 3.5.2.3   | ABAYE2577 OR ABAYE2646              | CAASP <=> DOROA                           | dihydroorotase  |
| R301 | Pyrimidine metabolism (De novo) | 1.3.3.1   | ABAYE1278                           | DOROA + UQ <=> UQH2 + OROA                | dihydroorotate oxidase  |
| R302 | Pyrimidine metabolism (De novo) | 1.3.3.1   | ABAYE1278                           | DOROA + MK <=> MKH2 + OROA                | dihydroorotate oxidase  |
| R303 | Pyrimidine metabolism (De novo) | 2.4.2.10  | ABAYE0144                           | OROA + PRPP <=> PPI + OMP                 | orotate phosphoribosyltransferase   |

| No.  | Metabolism                               | EC Number            | ORF                                   | Reaction   | Enzyme  |
|------|--|----------------------|---------------------------------------|--|---|
| R304 | Pyrimidine metabolism (De novo)          | 4.1.1.23             | ABAYE2058                             | OMP -> CO2 + UMP                                       | orotidine-5'-phosphate decarboxylase  |
| R305 | Pyrimidine metabolism (De novo)          | 2.7.4.6              | ABAYE3267                             | UDP + ATP <=> UTP + ADP                                | nucleoside-diphosphate kinase   |
| R306 | Pyrimidine metabolism (De novo)          | 6.3.4.2              | ABAYE1667                             | UTP + GLN + ATP -> GLU + CTP + ADP + PI                | CTP synthase  |
| R307 | Pyrimidine metabolism                    | 6.3.4.2              | ABAYE1667                             | ATP + UTP + NH3 -> ADP + PI + CTP                      | CTP synthase  |
| R308 | Pyrimidine metabolism                    | 2.7.4.6              | ABAYE3267                             | CDP + ATP <=> CTP + ADP                                | nucleoside-diphosphate kinase   |
| R309 | Pyrimidine metabolism                    | 1.17.4.1             | ABAYE3065 AND ABAYE3067               | CDP + RTHIO -> DCDP + OTHIO                            | ribonucleoside-diphosphate reductase  |
| R310 | Pyrimidine metabolism                    | 2.7.4.6              | ABAYE3267                             | DCDP + ATP <=> DCTP + ADP                              | nucleoside-diphosphate kinase   |
| R311 | Pyrimidine metabolism                    | 2.7.4.9              | ABAYE0933                             | DTMP + ATP <=> DTD + ADP                               | thymidylate kinase  |
| R312 | Pyrimidine metabolism                    | 2.7.4.6              | ABAYE3267                             | DTDP + ATP <=> DTTT + ADP                              | nucleoside-diphosphate kinase   |
| R313 | Pyrimidine metabolism                    | 2.7.4.14             | ABAYE2062                             | CMP + ATP <=> ADP + CDP                                | cytidylate kinase   |
| R314 | Pyrimidine metabolism                    | 1.8.1.9              | ABAYE2940 OR ABAYE3661                | OTHIO + NADPH -> RTHIO + NADP                          | thioredoxin reductase   |
| R315 | Pyrimidine metabolism                    | 2.7.4.14             | ABAYE2062                             | DCMP + ATP <=> ADP + DCDP                              | cytidylate kinase   |
| R316 | Pyrimidine metabolism                    | 2.4.2.9              | ABAYE3047                             | URA + PRPP <=> UMP + PPI                               | uracil phosphoribosyltransferase  |
| R317 | Pyrimidine metabolism                    | 4.2.1.70             | ABAYE1445                             | URA + R5P <=> PURI5P                                   | pseudouridylate synthase  |
| R318 | Pyrimidine metabolism                    | 2.1.1.45             | ABAYE3314                             | DUMP + METTHF -> DHF + DTMP                            | thymidylate synthase  |
| R319 | Pyrimidine metabolism                    | 2.4.2.1 OR 2.4.2.4   |                                       | DU + PI -> URA + DR1P                                  | purine-nucleoside phosphorylase OR thymidine phosphorylase                                  |
| R320 | Pyrimidine metabolism                    | 2.4.2.4              |                                       | DT + PI -> TM + DR1P                                   | thymidine phosphorylase   |
| R321 | Pyrimidine metabolism                    | 2.7.4.6              | ABAYE3267                             | DUDP + ATP <=> DUTP + ADP                              | nucleoside-diphosphate kinase   |
| R322 | Pyrimidine metabolism                    | 1.17.4.1             | ABAYE3065 AND ABAYE3067               | UDP + RTHIO -> OTHIO + DUDP                            | ribonucleoside-diphosphate reductase  |
| R323 | Pyrimidine metabolism                    | 2.7.4.9              | ABAYE0933                             | ATP + DUMP <=> ADP + DUDP                              | thymidylate kinase  |
| R324 | Pyrimidine metabolism                    | 3.1.3.5              | ABAYE1047 OR ABAYE1886                | UMP -> URI + PI  | 5'-nucleotidase   |
| R325 | Pyrimidine metabolism                    | 3.1.3.5              | ABAYE1047 OR ABAYE1886                | CMP -> CYTD + PI                                       | 5'-nucleotidase   |
| R326 | Pyrimidine metabolism                    | 3.1.3.5              | ABAYE1047 OR ABAYE1886                | DCMP -> DC + PI  | 5'-nucleotidase   |
| R327 | Pyrimidine metabolism                    | 3.1.3.5              | ABAYE1047 OR ABAYE1886                | DTMP -> DT + PI  | 5'-nucleotidase   |
| R328 | Pyrimidine metabolism                    | 3.5.4.1              |                                       | 5MC <=> TM + NH3                                       | cytosine deaminase  |
| R329 | Pyrimidine metabolism                    | 3.5.4.1              |                                       | CT -> URA + NH3  | cytosine deaminase  |
| R330 | Pyrimidine metabolism                    | 3.5.4.5              |                                       | DC -> DU + NH3   | cytidine deaminase  |
| R331 | Pyrimidine metabolism                    | 2.7.4.14 OR 2.7.4.22 | ABAYE2062 OR ABAYE1577                | ATP + UMP <=> ADP + UDP                                | cytidylate kinase OR uridylate kinase   |
| R332 | Pyrimidine metabolism                    | 3.5.4.13             | ABAYE3025                             | CTP -> UTP + NH3                                       | deoxycytidine triphosphate deaminase  |
| R333 | Pyrimidine metabolism                    | 3.5.4.13             | ABAYE3025                             | DCTP -> DUTP + NH3                                     | deoxycytidine triphosphate deaminase  |
| R334 | Pyrimidine metabolism                    | 3.6.1.19             | ABAYE3179                             | UTP -> UMP + PPI                                       | nucleoside-triphosphate pyrophosphatase   |
| R335 | Pyrimidine metabolism                    | 3.6.1.19 OR 3.6.1.23 | ABAYE3179 OR ABAYE2929                | DUTP -> DUMP + PPI                                     | nucleoside-triphosphate pyrophosphatase OR deoxyuridine 5'-triphosphate nucleotidohydrolase |
| R336 | Glutamate metabolism                     | 6.3.1.2              | ABAYE1126 OR ABAYE1425                | GLU + NH3 + ATP -> GLN + ADP + PI                      | glutamine synthetase  |
| R337 | Glutamate metabolism                     | 1.4.1.13 OR 1.4.1.14 | ABAYE0298 AND ABAYE0299               | GLN + AKG + NADPH -> 2 GLU + NADP                      | glutamate synthase  |
| R338 | Glutamate metabolism                     | 6.3.5.5              | ABAYE0800 AND ABAYE0801               | GLN + 2 ATP + HCO3 -> GLU + CAP + 2 ADP + PI           | carbamoyl-phosphate synthase  |
| R339 | Glutamate metabolism                     | 6.1.1.17             | ABAYE0277                             | TRNAGLU + GLU + ATP -> GLUTRAGLU + PPI + AMP           | glutamyl-tRNA synthetase  |
| R340 | Glutamate metabolism                     | 6.1.1.18             | ABAYE1455                             | ATP + GLN + TRNAGLN -> AMP + PPI + GTRNA               | glutaminyl-tRNA synthetase  |
| R341 | Glutamate metabolism                     | 3.5.1.2 OR 3.5.1.38  | ABAYE2832 OR ABAYE2188                | GLN -> GLU + NH3                                       | glutaminase OR glutaminase-asparaginase   |
| R342 | Glutamate metabolism                     | 6.3.5.7              | ABAYE0697 AND ABAYE0698 AND ABAYE0699 | GTRNA + GLU + PI + ADP <=> GLUTRAGLN + GLN + ATP       | aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase  |
| R343 | Alanine and aspartate metabolism         | 2.6.1.1              | ABAYE0951                             | OA + GLU <=> ASP + AKG                                 | aspartate aminotransferase  |
| R344 | Alanine and aspartate metabolism         | 6.1.1.12             | ABAYE0588                             | ATP + ASP + TRNAASP -> AMP + PPI + ASPTRNAASP          | aspartyl-tRNA synthetase  |
| R345 | Alanine and aspartate metabolism         | 6.1.1.7              | ABAYE2595                             | ATP + ALA + TRNAALA <=> AMP + PPI + ALATRNA            | alanyl-tRNA synthetase  |
| R346 | Alanine and aspartate metabolism         | 6.3.5.4              |                                       | ASP + ATP + GLN -> GLU + ASN + AMP + PPI               | asparagine synthase   |
| R347 | Alanine and aspartate metabolism         | 3.5.1.1 OR 3.5.1.38  | ABAYE3351 OR ABAYE2188                | ASN -> ASP + NH3                                       | L-asparaginase I OR glutaminase-asparaginase  |
| R348 | Alanine and aspartate metabolism         | 3.4.13.3             | ABAYE1209                             | CNS -> bALA + HIS                                      | aminoacyl-histidine dipeptidase (peptidase D)   |
| R349 | Alanine and aspartate metabolism         | 1.4.3.16             | ABAYE0935                             | ASP + O2 -> OA + NH3 + H2O2                            | L-aspartate oxidase   |
| R350 | Alanine and aspartate metabolism         | 5.1.1.13             | ABAYE1354                             | ASP <=> DASP   | aspartate/glutamate racemase  |
| R351 | Alanine and aspartate metabolism         | 6.3.5.6              | ABAYE0697 AND ABAYE0698 AND ABAYE0699 | ASNTRNAASN + GLU + PI + ADP <=> ASPTRNAASN + GLN + ATP | aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase  |
| R352 | Glycine, serine and threonine metabolism | 2.7.2.4              | ABAYE2596                             | ASP + ATP -> ADP + BASP                                | aspartate kinase  |
| R353 | Glycine, serine and threonine metabolism | 1.2.1.11             | ABAYE3348                             | BASP + NADPH -> NADP + PI + ASPSA                      | aspartate-semialdehyde dehydrogenase  |
| R354 | Glycine, serine and threonine metabolism | 1.1.1.3              | ABAYE1937 OR ABAYE3530                | ASPSA + NADH <=> NAD + HSER                            | homoserine dehydrogenase  |
| R355 | Glycine, serine and threonine metabolism | 1.1.1.3              | ABAYE1937 OR ABAYE3530                | ASPSA + NADPH <=> NADP + HSER                          | homoserine dehydrogenase  |
| R356 | Glycine, serine and threonine metabolism | 2.7.1.39             | ABAYE0244                             | HSER + ATP -> ADP + PHSER                              | homoserine kinase   |
| R357 | Glycine, serine and threonine metabolism | 4.2.3.1              | ABAYE3531                             | PHSER -> THR + PI                                      | threonine synthase  |
| R358 | Glycine, serine and threonine metabolism | 1.1.1.95             | ABAYE0332                             | 3PG + NAD -> NADH + PHP                                | D-3-phosphoglycerate dehydrogenase  |
| R359 | Glycine, serine and threonine metabolism | 2.6.1.52             | ABAYE0877                             | PHP + GLU -> AKG + 3PSER                               | phosphoserine aminotransferase  |
| R360 | Glycine, serine and threonine metabolism | 3.1.3.3              | ABAYE0098                             | 3PSER -> PI + SER                                      | phosphoserine phosphatase   |
| R361 | Glycine, serine and threonine metabolism | 2.1.2.1              | ABAYE1171                             | THF + SER <=> GLY + METTHF                             | serine hydroxymethyltransferase   |

| No.  | Metabolism                                 | EC Number             | ORF   | Reaction   | Enzyme   |
|------|--|-----------------------|---|--|--|
| R362 | Glycine, serine and threonine metabolism   | 1.8.1.4               | ABAYE0505 OR ABAYE0782 OR ABAYE1945   | DHLIPOYLPROTEIN + NAD -> NADH + LIPOYLPROTEIN        | dihydroliipoamide dehydrogenase  |
| R363 | Glycine, serine and threonine metabolism   | 4.3.1.17 OR 4.3.1.19  | ABAYE2377 OR (ABAYE0691 OR ABAYE1083 OR ABAYE1649)  | SER <-> PYR + NH3                                    | L-serine ammonia-lyase   |
| R364 | Glycine, serine and threonine metabolism   | 4.3.1.19              | ABAYE0691 OR ABAYE1083 OR ABAYE1649   | THR -> OBUT + NH3                                    | threonine dehydratase  |
| R365 | Glycine, serine and threonine metabolism   | 6.1.1.3               | ABAYE3169   | ATP + THR + TRNATHR -> AMP + PPI + THRTRNATHR        | threonyl-tRNA synthetase   |
| R366 | Glycine, serine and threonine metabolism   | 6.1.1.11              | ABAYE0757   | ATP + SER + TRNASER -> AMP + PPI + SERTRNASER        | seryl-tRNA synthetase  |
| R367 | Glycine, serine and threonine metabolism   | 6.1.1.14              | ABAYE0367 AND ABAYE0368   | ATP + GLY + TRNAGLY -> AMP + PPI + GLYTRNAGLY        | glycyl-tRNA synthetase   |
| R368 | Glycine, serine and threonine metabolism   | 2.6.1.76              | ABAYE1026   | GLU + ASPSA -> AKG + 24DAB                           | glutamate decarboxylase  |
| R369 | Glycine, serine and threonine metabolism   | 1.1.99.1              | ABAYE2868   | BAL + FAD -> FADH2 + BETAINE                         | choline dehydrogenase  |
| R370 | Glycine, serine and threonine metabolism   | 1.2.1.8               | ABAYE1066 OR ABAYE2867  | BAL + NAD -> BETAINE + NADH                          | NAD-dependent aldehyde dehydrogenase   |
| R371 | Glycine, serine and threonine metabolism   | 1.1.1.-               | ABAYE0043 OR ABAYE0109 OR ABAYE0479 OR ABAYE1356 OR ABAYE2589 OR ABAYE2607 OR ABAYE2613 OR ABAYE2618 OR ABAYE2845 OR ABAYE3187 OR ABAYE3378                           | MTG + NADPH -> HAC + NADP                            | alcohol dehydrogenase  |
| R372 | Glycine, serine and threonine metabolism   | 1.4.3.21              | ABAYE1710   | AACTN + O2 <-> MTG + NH3 + H2O2                      | copper amine oxidase precursor (tyramine oxidase) (2-phenylethylamine oxidase) |
| R373 | Glycine, serine and threonine metabolism   | 4.3.1.18              | ABAYE2819   | DSEER <-> PYR + NH3                                  | D-serine deaminase (dehydratase)   |
| R374 | Methionine metabolism                      | 4.4.1.8               | ABAYE0405   | LLCT -> HCYS + PYR + NH3                             | cystathionine beta-lyase, PLP-dependent  |
| R375 | Methionine metabolism                      | 2.1.1.13              | ABAYE2822   | HCYS + MTHF <-> THF + MET                            | methionine synthase I  |
| R376 | Methionine metabolism                      | 2.1.1.14              | ABAYE3079   | 5MTGLU + HCYS -> TGLU + MET                          | 5-methyltetrahydropteroylglutamate-homocysteine methyltransferase              |
| R377 | Methionine metabolism                      | 6.1.1.10              | ABAYE3031   | ATP + MET + TRNAMET -> AMP + PPI + METTRNA           | methionyl-tRNA synthetase  |
| R378 | Methionine metabolism                      | 2.1.2.9               | ABAYE0022   | METTRNA + FTHF -> THF + FMETTRNA                     | methionyl-tRNA formyltransferase   |
| R379 | Methionine metabolism                      | 2.5.1.6               | ABAYE2118   | MET + ATP -> PPI + PI + SAM                          | S-adenosylmethionine synthetase  |
| R380 | Methionine metabolism                      | 3.2.2.9               | ABAYE3028 OR ABAYE3846  | SAH <-> SRLH + AD                                    | S-adenosylhomocysteine nucleosidase  |
| R381 | Methionine metabolism                      | 2.1.1.37              | ABAYE0084   | SAM + CT <-> SAH + 5MC                               | cytosine-specific methyltransferase  |
| R382 | Methionine metabolism                      | 2.3.1.31              | ABAYE3293   | ACCOA + HSER <-> COA + OAHSER                        | homoserine O-acetyltransferase   |
| R383 | Methionine metabolism                      | 2.5.1.-               | ABAYE1970   | OSLHSEER + H2S <-> HCYS + SUCC                       | O-succinylhomoserine sulphydrylase   |
| R384 | Methionine metabolism                      | 2.5.1.49              | ABAYE0264   | OAHSER + H2S <-> HCYS + AC                           | homocysteine synthase  |
| R385 | Methionine metabolism                      | 2.5.1.49              | ABAYE0264   | OAHSER + HO3S2 + RTHIO <-> HCYS + H2SO3 + OTHIO + AC | homocysteine synthase  |
| R386 | Cysteine metabolism                        | 4.4.1.8               | ABAYE0405   | H2S + PYR + NH3 -> CYS                               | cystathionine beta-lyase   |
| R387 | Cysteine metabolism                        | 4.4.1.8               | ABAYE0405   | CYST -> PYR + NH3 + TCYS                             | cystathionine beta-lyase   |
| R388 | Cysteine metabolism                        | 2.3.1.30              | ABAYE2191 OR ABAYE2248  | SER + ACCCOA <-> COA + ASER                          | serine acetyltransferase   |
| R389 | Cysteine metabolism                        | 2.5.1.47              | ABAYE3184 OR ABAYE3696  | ASER + H2S -> CYS + AC                               | cysteine synthase  |
| R390 | Cysteine metabolism                        | 2.5.1.47 OR 2.5.1.49  | ABAYE3184 OR ABAYE3696 OR ABAYE0264   | ASER + HO3S2 + RTHIO -> CYS + H2SO3 + OTHIO + AC     | cysteine synthase  |
| R391 | Cysteine metabolism                        | 2.5.1.47              | ABAYE3184 OR ABAYE3696  | ASER + HO3S2 -> SSLCYS + AC                          | cysteine synthase  |
| R392 | Cysteine metabolism                        | 2.6.1.1               | ABAYE0951   | CYSTEATE + AKG <-> 3SPYR + GLU                       | aspartate aminotransferase   |
| R393 | Cysteine metabolism                        | 2.6.1.1               | ABAYE0951   | 3SLALA + AKG -> 3SFPYR + GLU                         | aspartate aminotransferase   |
| R394 | Cysteine metabolism                        | 2.6.1.1               | ABAYE0951   | MPYR + GLU -> CYS + AKG                              | aspartate aminotransferase   |
| R395 | Cysteine metabolism                        | 4.3.1.17              | ABAYE2377   | SER -> 2AA   | L-serine dehydratase   |
| R396 | Cysteine metabolism                        | 6.1.1.16              | ABAYE2493   | ATP + CYS + TRNACYS -> AMP + PPI + CYSTRNACYS        | cysteinyl-tRNA synthetase  |
| R397 | Cysteine metabolism                        | 4.4.1.15              | ABAYE3037   | DCYS <-> H2S + NH3 + PYR                             | D-cysteine desulhydrase  |
| R398 | Valine, leucine and isoleucine degradation | 1.1.1.31              | ABAYE3767   | HIBUT + NAD -> 3OPP + NADH                           | 3-hydroxyisobutyrate dehydrogenase   |
| R399 | Valine, leucine and isoleucine degradation | 1.3.99.3 OR 1.3.99.10 | (ABAYE0476 OR ABAYE2013) OR ABAYE2288   | 3MBCOA + FAD <-> 3MCCOA + FADH2                      | acyl-CoA dehydrogenase   |
| R400 | Valine, leucine and isoleucine degradation | 4.2.1.17              | ABAYE0482 OR ABAYE0915 OR ABAYE2065 OR ABAYE2290 OR ABAYE2304 OR ABAYE2311 OR ABAYE2369 OR ABAYE2370 OR ABAYE2628 OR ABAYE2852 OR ABAYE3186 OR ABAYE3763 OR ABAYE3764 | 3HIVCOA <-> 3MCCOA                                   | enoyl-CoA hydratase  |
| R401 | Valine, leucine and isoleucine degradation | 4.2.1.17              | ABAYE0482 OR ABAYE0915 OR ABAYE2065 OR ABAYE2290 OR ABAYE2304 OR ABAYE2311 OR ABAYE2369 OR ABAYE2370 OR ABAYE2628 OR ABAYE2852 OR ABAYE3186 OR ABAYE3763 OR ABAYE3764 | 2MP2Ecoa -> 3HIBCOA                                  | enoyl-CoA hydratase  |

| No.  | Metabolism                                  | EC Number  | ORF   | Reaction                                       | Enzyme  |
|------|---|------------|---|--|---|
| R402 | Valine, leucine and isoleucine degradation  | 4.2.1.17   | ABAYE0482 OR<br>ABAYE0915 OR<br>ABAYE2065 OR<br>ABAYE2290 OR<br>ABAYE2304 OR<br>ABAYE2311 OR<br>ABAYE2369 OR<br>ABAYE2370 OR<br>ABAYE2628 OR<br>ABAYE2852 OR<br>ABAYE3186 OR<br>ABAYE3763 OR<br>ABAYE3764 | 3H2MBCOA -> 2MB2ECO A                          | enoyl-CoA hydratase   |
| R403 | Valine, leucine and isoleucine degradation  | 6.4.1.4    | ABAYE0483   | ATP + 3MCCOA + HCO3 -> ADP + Pi + 3MGCOA       | 3-methylcrotonyl-CoA carboxylase  |
| R404 | Valine, leucine and isoleucine degradation  | 1.1.1.35   | ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470   | HIBUT + NAD <-> MMSA + NADH                    | 3-hydroxyacyl-CoA dehydrogenase   |
| R405 | Valine, leucine and isoleucine degradation  | 1.1.1.35   | ABAYE1411 OR<br>ABAYE2460 OR<br>ABAYE3470   | 3H2MBCOA + NAD <-> 2MAACCOA + NADH             | 3-hydroxyacyl-CoA dehydrogenase   |
| R406 | Valine, leucine and isoleucine degradation  | 1.2.1.3    | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | MMSA + NAD -> MM + NADH                        | aldehyde dehydrogenase  |
| R407 | Valine, leucine and isoleucine degradation  | 2.3.1.16   | ABAYE3471   | COA + 2MAACCOA -> PPACOA + ACCOA               | acetyl-CoA acyltransferase  |
| R408 | Valine, leucine and isoleucine degradation  | 1.3.99.3   | ABAYE0476 OR<br>ABAYE2013   | 2MPACOA + FAD <-> 2MP2ECO A + FADH2            | acyl-CoA dehydrogenase  |
| R409 | Valine, leucine and isoleucine degradation  | 1.3.99.3   | ABAYE0476 OR<br>ABAYE2013   | 2MBCOA + FAD <-> 2MB2ECO A + FADH2             | acyl-CoA dehydrogenase  |
| R410 | Valine, leucine and isoleucine degradation  | 2.6.1.18   | ABAYE1295   | ALA + MMSA <-> PYR + AIBUT                     | omega-amino acid-pyruvate aminotransferase (omega-APT) (beta-alanine-pyruvate aminotransferase) |
| R411 | Valine, leucine and isoleucine degradation  | 2.6.1.42   | ABAYE0577   | ILE + AKG <-> 3MOP + GLU                       | branched-chain amino acid transferase   |
| R412 | Valine, leucine and isoleucine degradation  | 2.6.1.42   | ABAYE0577   | LEU + AKG <-> 4MOP + GLU                       | branched-chain amino acid transferase   |
| R413 | Valine, leucine and isoleucine biosynthesis | 1.1.1.86   | ABAYE3238   | ACLAC + NADPH -> NADP + DHMVA                  | acetohydroxy acid isomeroreductase  |
| R414 | Valine, leucine and isoleucine biosynthesis | 4.2.1.9    | ABAYE0023 OR<br>ABAYE1724 OR<br>ABAYE1781   | DHMVA -> OIVAL                                 | dihydroxy-acid dehydratase OR 6-phosphogluconate dehydratase                                    |
| R415 | Valine, leucine and isoleucine biosynthesis | 2.6.1.42   | ABAYE0577   | OIVAL + GLU <-> AKG + VAL                      | branched-chain amino acid aminotransferase  |
| R416 | Valine, leucine and isoleucine biosynthesis | 2.2.1.6    | ABAYE2836 OR<br>(ABAYE3239 AND<br>ABAYE3240)  | OBUT + 2(HE)TPP -> ABUT + THMPP                | acetolactate synthase   |
| R417 | Valine, leucine and isoleucine biosynthesis | 1.1.1.86   | ABAYE3238   | ABUT + NADPH -> NADP + DHMP                    | ketol-acid reductoisomerase   |
| R418 | Valine, leucine and isoleucine biosynthesis | 4.2.1.9    | ABAYE0023 OR<br>ABAYE1724 OR<br>ABAYE1781   | DHMP -> 3MOP                                   | dihydroxy-acid dehydratase  |
| R419 | Valine, leucine and isoleucine biosynthesis | 2.6.1.42   | ABAYE0577   | 3MOP + GLU <-> AKG + ILE                       | branched-chain amino acid aminotransferase  |
| R420 | Valine, leucine and isoleucine biosynthesis | 2.3.3.13   | ABAYE3292   | ACCOA + OIVAL -> COA + IPPMAL                  | isopropylmalate synthase  |
| R421 | Valine, leucine and isoleucine biosynthesis | 4.2.1.33   | ABAYE3359 AND<br>ABAYE3360  | IPPMAL <-> CBHCAP                              | 3-isopropylmalate dehydratase   |
| R422 | Valine, leucine and isoleucine biosynthesis | 1.1.1.85   | ABAYE3357   | CBHCAP + NAD -> NADH + OICAP                   | isopropylmalate dehydrogenase   |
| R423 | Valine, leucine and isoleucine biosynthesis |            |   | OICAP -> 4MOP + CO2                            | spontaneous   |
| R424 | Valine, leucine and isoleucine biosynthesis | 2.6.1.42   | ABAYE0577   | 4MOP + GLU <-> AKG + LEU                       | branched-chain amino acid aminotransferase  |
| R425 | Valine, leucine and isoleucine biosynthesis | 6.1.1.4    | ABAYE3244   | ATP + LEU + TRNALEU -> AMP + PPI + LEUTRNA     | leucyl-tRNA synthetase  |
| R426 | Valine, leucine and isoleucine biosynthesis | 6.1.1.9    | ABAYE0740   | ATP + VAL + TRNAVAL -> AMP + PPI + VALTRNAVAL  | valyl-tRNA synthetase   |
| R427 | Valine, leucine and isoleucine biosynthesis | 6.1.1.5    | ABAYE3852   | ATP + ILE + TRNAILE -> AMP + PPI + ILETRNAILE  | isoleucyl-tRNA synthetase   |
| R428 | Lysine biosynthesis                         | 4.2.1.52   | ABAYE0058 OR<br>ABAYE2388 OR<br>ABAYE2878 OR<br>ABAYE3671   | ASPSA + PYR -> DHDP                            | dihydrodipicolinate synthase  |
| R429 | Lysine biosynthesis                         | 1.3.1.26   | ABAYE0036   | DHDP + NADPH -> NADP + TDHDP                   | dihydrodipicolinate reductase   |
| R430 | Lysine biosynthesis                         | 1.3.1.26   | ABAYE0036   | DHDP + NADH -> NAD + TDHDP                     | dihydrodipicolinate reductase   |
| R431 | Lysine biosynthesis                         | 2.3.1.117  | ABAYE0923   | TDHDP + SUCCOA -> SAOPI M + COA                | 2,3,4,5-tetrahydropyridine-2,6-carboxylate N-succinyltransferase                                |
| R432 | Lysine biosynthesis                         | 2.6.1.17   | ABAYE2181   | SAOPI M + GLU -> SDAPIM + AKG                  | succinyl-diaminopimelate transaminase   |
| R433 | Lysine biosynthesis                         | 3.5.1.18   | ABAYE0676   | SDAPIM -> DAPIM + SUCC                         | succinyl-diaminopimelate desuccinylase  |
| R434 | Lysine biosynthesis                         | 5.1.1.7    | ABAYE0861   | DAPIM <-> MDAPIM                               | diaminopimelate epimerase   |
| R435 | Lysine biosynthesis                         | 4.1.1.20   | ABAYE0860   | MDAPIM -> LYS + CO2                            | diaminopimelate decarboxylase   |
| R436 | Lysine biosynthesis                         | 6.1.1.6    | ABAYE0854 OR<br>ABAYE2794   | ATP + LYS + TRNALYS -> AMP + PPI + LYSTRNA     | lysyl-tRNA synthetase   |
| R437 | Lysine biosynthesis                         | 1.1.1.3    | ABAYE1937 OR<br>ABAYE3530   | HSER + NAD <-> ASPSA + NADH                    | homoserine dehydrogenase  |
| R438 | Lysine biosynthesis                         | 1.1.1.3    | ABAYE1937 OR<br>ABAYE3530   | HSER + NADP <-> ASPSA + NADPH                  | homoserine dehydrogenase  |
| R439 | Lysine biosynthesis                         | 1.2.1.11   | ABAYE3348   | ASPSA + PI + NADP <-> BASP + NADPH             | aspartate-semialdehyde dehydrogenase  |
| R440 | Lysine degradation                          | 1.2.4.2    | ABAYE0780   | 2OAD + LIPO -> SGDHL + CO2                     | 2-oxoglutarate dehydrogenase E1 component   |
| R441 | Lysine degradation                          | 2.3.1.61   | ABAYE0781   | GLUTCOA + DLIPO <-> COA + SGDHL                | 2-oxoglutarate dehydrogenase E2 component   |
| R442 | Lysine degradation                          | 1.14.13.59 | ABAYE1094   | LYS + O2 + NADPH <-> NHLYS + NADP              | acinetobactin siderophore biosynthesis protein OR lysine N6-hydroxylase                         |
| R443 | Lysine degradation                          | 1.2.1.3    | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | 4TMABT + NAD <-> 4TMABTO + NADH                | aldehyde dehydrogenase  |
| R444 | Lysine degradation                          | 1.3.99.7   | ABAYE3097   | GLUTCOA <-> CCOA + CO2                         | glutaryl-CoA dehydrogenase  |
| R445 | Arginine and proline metabolism             | 2.3.1.109  | ABAYE0353   | SUCCOA + ARG -> COA + N2SUCCARG                | arginine succinyltransferase  |
| R446 | Arginine and proline metabolism             | 6.1.1.19   | ABAYE3732   | ATP + ARG + TRNAARG <-> AMP + PPI + ARGTRNAARG | arginyl-tRNA synthetase   |
| R447 | Arginine and proline metabolism             | 1.5.1.12   | ABAYE2108   | P5C + NAD -> NADH + GLU                        | bifunctional proline dehydrogenase OR delta-1-pyrroline-5-carboxylate dehydrogenase             |

| No.  | Metabolism                      | EC Number            | ORF  | Reaction                                      | Enzyme   |
|------|---------------------------------|----------------------|--|---|--|
| R448 | Arginine and proline metabolism | 1.5.1.12             | ABAYE2108  | P5C + NADP -> NADPH + GLU                     | bifunctional proline dehydrogenase OR delta-1-pyrroline-5-carboxylate dehydrogenase  |
| R449 | Arginine and proline metabolism | 1.5.1.12             | ABAYE2108  | GLUGSAL + NAD -> NADH + GLU                   | 1-pyrroline-5-carboxylate dehydrogenase  |
| R450 | Arginine and proline metabolism | 1.5.99.8             | ABAYE2108  | PRO + FAD -> P5C + FADH2                      | proline dehydrogenase  |
| R451 | Arginine and proline metabolism | 6.1.1.15             | ABAYE0663  | ATP + PRO + TRNAPRO -> AMP + PPI + PROTRNAPRO | prolyl-tRNA synthetase   |
| R452 | Arginine and proline metabolism | 1.5.1.2              | ABAYE2533 OR ABAYE3151   | L1P3H5C + NADH -> 4HPRO + NAD                 | pyrroline-5-carboxylate reductase  |
| R453 | Arginine and proline metabolism | 1.5.1.2              | ABAYE2533 OR ABAYE3151   | L1P3H5C + NADPH -> 4HPRO + NADP               | pyrroline-5-carboxylate reductase  |
| R454 | Arginine and proline metabolism | 1.5.1.12             | ABAYE2108  | L1P3H5C + NAD -> E4HGLU + NADH                | 1-pyrroline-5-carboxylate dehydrogenase  |
| R455 | Arginine and proline metabolism | 1.5.1.12             | ABAYE2108  | L1P3H5C + NADP -> E4HGLU + NADPH              | 1-pyrroline-5-carboxylate dehydrogenase  |
| R456 | Arginine and proline metabolism | 1.5.1.12 OR 1.5.99.8 | ABAYE2108  | E4HGLU + NAD <-> 4HGLUSA + NADH               | 1-pyrroline-5-carboxylate dehydrogenase  |
| R457 | Arginine and proline metabolism | 2.6.1.1              | ABAYE0951  | E4HGLU + AKG -> HYDROXYAKG + GLU              | aspartate aminotransferase   |
| R458 | Arginine and proline metabolism | 4.1.2.14             | ABAYE3280  | HYDROXYAKG <-> PYR + GLX                      | 4-hydroxy-2-oxoglutarate aldolase  |
| R459 | Arginine and proline metabolism | 1.2.1.71             | ABAYE0354  | N2SUCCGLU5SA + NAD -> N2SUCCGLU + NADH        | succinylglutamic semialdehyde dehydrogenase  |
| R460 | Arginine and proline metabolism | 2.6.1.81             | ABAYE0352  | SORN + AKG -> N2SUCCGLU5SA + GLU              | succinylornithine transaminase   |
| R461 | Arginine and proline metabolism | 3.5.1.96             | ABAYE0356  | N2SUCCGLU -> GLU + SUCC                       | succinylglutamate desuccinylase  |
| R462 | Arginine and proline metabolism | 3.5.3.23             | ABAYE0355  | N2SUCCARG -> SORN + CO2 + 2 NH3               | succinylarginine dihydrolase   |
| R463 | Arginine and proline metabolism | 3.5.3.3              | p3ABAYE0029  | CRTN <-> SCSN + UREA                          | creatinase (Creatine aminohydrolase)   |
| R464 | Arginine and proline metabolism | 5.1.1.4              | ABAYE2385  | PRO <-> DPRO                                  | proline racemase   |
| R465 | Histidine metabolism            | 2.4.2.17             | ABAYE2593 OR ABAYE3132   | PRPP + ATP -> PPI + PRBAMP                    | ATP phosphoribosyltransferase  |
| R466 | Histidine metabolism            | 3.6.1.31             | ABAYE3428  | PRBAMP -> PPI + PRBAMP                        | phosphoribosyl-ATP pyrophosphohydrolase  |
| R467 | Histidine metabolism            | 3.5.4.19             | ABAYE3428  | PRBAMP -> PRFP                                | phosphoribosyl-AMP cyclohydrolase  |
| R468 | Histidine metabolism            | 5.3.1.16             | ABAYE0250  | PRFP -> PRLP                                  | phosphoribosylformimino-5-aminoimidazole carboxamide ribotide isomerase  |
| R469 | Histidine metabolism            | 2.4.2.- OR 4.1.3.-   | ABAYE0243 OR ABAYE0253   | PRLP + GLN -> GLU + AICAR + DIMGP             | imidazole glycerol phosphate synthase OR glutamine amidotransferase  |
| R470 | Histidine metabolism            | 4.2.1.19             | ABAYE0254  | DIMGP -> IMACP                                | imidazoleglycerol-phosphate dehydratase  |
| R471 | Histidine metabolism            | 2.6.1.9              | ABAYE3130  | IMACP + GLU -> AKG + HISOLP                   | histidinol-phosphate aminotransferase  |
| R472 | Histidine metabolism            | 3.1.3.15             |  | HISOLP -> PI + HISOL                          | histidinol-phosphatase   |
| R473 | Histidine metabolism            | 1.1.1.23             | ABAYE3131  | HISOL + 2 NAD -> HIS + 2 NADH                 | histidinol dehydrogenase   |
| R474 | Histidine metabolism            | 2.1.1.-              | ABAYE0624 OR ABAYE2481 OR ABAYE2566 OR ABAYE2771 OR ABAYE2871  | HIS + SAM -> NMHIS + SAH                      | N6-adenine-specific methylase  |
| R475 | Histidine metabolism            | 6.1.1.21             | ABAYE3262  | ATP + HIS + TRNAHIS -> AMP + PPI + HISTRNAHIS | histidyl-tRNA synthetase   |
| R476 | Histidine metabolism            | 4.3.1.3              | ABAYE0076  | HIS -> UC + NH3                               | histidine ammonia-lyase  |
| R477 | Histidine metabolism            | 4.2.1.49             | ABAYE0075  | UC -> 4I5P                                    | urocanate hydratase  |
| R478 | Histidine metabolism            | 3.5.2.7              | ABAYE0078  | 4I5P -> NFGLU                                 | imidazolonepropionase  |
| R479 | Histidine metabolism            | 3.5.3.8              | ABAYE0079  | NFGLU -> GLU + FA                             | formiminoglutamate   |
| R480 | Histidine metabolism            | 1.2.1.3              | ABAYE1028 OR ABAYE1460 OR ABAYE2333 OR ABAYE2837   | I4AA + NAD -> I4AC + NADH                     | aldehyde dehydrogenase   |
| R481 | Histidine metabolism            | 1.14.13.-            | ABAYE0129 OR ABAYE0435 OR ABAYE2606 OR ABAYE2614   | 2 H5P <-> O2 + 2 4I5P                         | flavin-binding family monooxygenase  |
| R482 | Histidine metabolism            | 4.1.1.22             | ABAYE1098  | HIS <-> HIEA + CO2                            | histidine decarboxylase  |
| R483 | Tyrosine metabolism             | 5.3.3.10             | ABAYE1465  | 5CM2HM -> 5C2O3E                              | 5-carboxymethyl-2-hydroxymuconate isomerase  |
| R484 | Tyrosine metabolism             | 2.6.1.1              | ABAYE0951  | AKG + TYR <-> 4HPP + GLU                      | aspartate aminotransferase   |
| R485 | Tyrosine metabolism             | 1.13.11.27           | ABAYE0064  | 4HPP + O2 -> HOMOGEN + CO2                    | 4-hydroxyphenylpyruvate dioxygenase  |
| R486 | Tyrosine metabolism             | 5.2.1.2              | ABAYE0067  | 4MAAC -> 4FAAC                                | maleylacetoacetate isomerase   |
| R487 | Tyrosine metabolism             | 1.1.1.1              | ABAYE0763 OR ABAYE1463 OR ABAYE1522 OR ABAYE1861 OR p2ABAYE0004 OR p3ABAYE0020 OR p3ABAYE0024  | 34DHPEG + NAD <-> 34DHMA + NADH               | alcohol dehydrogenase  |
| R488 | Tyrosine metabolism             | 1.14.13.-            | ABAYE0129 OR ABAYE0435 OR ABAYE2606 OR ABAYE2614   | TRM + O2 + NADH <-> DPM + NAD                 | flavin-binding family monooxygenase  |
| R489 | Tyrosine metabolism             | 1.14.13.-            | ABAYE0129 OR ABAYE0435 OR ABAYE2606 OR ABAYE2614   | 4HPACALO + NADPH + O2 <-> 4HMN + NADP         | flavin-binding family monooxygenase  |
| R490 | Tyrosine metabolism             | 1.14.13.3            | ABAYE3078  | 3HPA + O2 + NADH <-> 34DHPA + NAD             | flavoprotein oxidoreductase  |
| R491 | Tyrosine metabolism             | 1.14.13.3            | ABAYE3078  | 4HPA + O2 + NADH <-> 34DHPA + NAD             | flavoprotein oxidoreductase  |
| R492 | Tyrosine metabolism             | 1.4.3.21             | ABAYE1710  | TRM + O2 <-> 4HPACAL + NH3 + H2O2             | copper amine oxidase precursor (tyramine oxidase) (2-phenylethylamine oxidase)   |
| R493 | Tyrosine metabolism             | 1.4.3.21             | ABAYE1710  | DPM + O2 <-> DHPACAL + NH3 + H2O2             | copper amine oxidase precursor (tyramine oxidase) (2-phenylethylamine oxidase)   |
| R494 | Tyrosine metabolism             | 2.1.1.-              | ABAYE0624 OR ABAYE2481 OR ABAYE2566 OR ABAYE2771 OR ABAYE2871  | MTRM + SAM <-> HDN + SAH                      | O-methyltransferase protein  |
| R495 | Tyrosine metabolism             | 2.3.1.-              | ABAYE0497 OR ABAYE0625 OR ABAYE1513 OR ABAYE1675 OR ABAYE1715 OR ABAYE1811 OR ABAYE2153 OR ABAYE2367 OR ABAYE2457 OR ABAYE2483 OR ABAYE3572 OR ABAYE3588 OR ABAYE3697 OR ABAYE3807 | 4HPACOA + GLY <-> 4HPAGLY + COA               | acyltransferase OR acetyl transferase OR acyl-CoA thiolase OR beta-ketoadipyl CoA thiolase OR GCN5-related N-acetyltransferase |
| R496 | Tyrosine metabolism             | 2.6.1.9 OR 2.6.1.57  | ABAYE3130 OR ABAYE3795   | TYR + AKG <-> 4HPP + GLU                      | histidinol-phosphate aminotransferase OR tyrosine aminotransferase   |
| R497 | Tyrosine metabolism             | 3.7.1.2              | ABAYE0068  | AAC + FUM <-> 4FAAC                           | fumarylacetoacetase (fumarylacetoacetate hydrolase)  |
| R498 | Tyrosine metabolism             | 4.1.1.-              | ABAYE1027  | HOMOGEN + O2 + NADPH <-> GENAL + CO2 + NADP   | L-2,4-diaminobutyrate decarboxylase  |



| No.  | Metabolism  | EC Number                            | ORF   | Reaction                                      | Enzyme   |
|------|---|--------------------------------------|---|---|--|
| R499 | Tyrosine metabolism                                 | 4.1.1.-                              | ABAYE1027   | DHI + CO2 <-> CDHDI                           | L-2,4-diaminobutyrate decarboxylase  |
| R500 | Tyrosine metabolism                                 | 4.1.1.-                              | ABAYE1027   | DPCHR <-> DHI + CO2                           | L-2,4-diaminobutyrate decarboxylase  |
| R501 | Phenylalanine metabolism                            | 2.6.1.1 OR<br>2.6.1.9 OR<br>2.6.1.57 | ABAYE0951<br>OR ABAYE3130 OR<br>ABAYE3795   | PHE + AKG <-> PHPYR + GLU                     | aspartate aminotransferase   |
| R502 | Phenylalanine metabolism                            | 1.13.11.27                           | ABAYE0064   | PHPYR + O2 -> 2HPA + CO2                      | 4-hydroxyphenylpyruvate dioxygenase  |
| R503 | Phenylalanine metabolism                            | 1.4.99.1                             | ABAYE1567 OR<br>ABAYE3774   | DPHE + FAD -> PHPYR + FADH2 + NH3             | D-amino-acid dehydrogenase   |
| R504 | Phenylalanine metabolism                            | 1.11.1.7                             | ABAYE0619   | PHE <-> PAA                                   | antioxidant protein  |
| R505 | Phenylalanine metabolism                            | 1.14.13.-                            | ABAYE0129 OR<br>ABAYE0435 OR<br>ABAYE2606 OR<br>ABAYE2614   | 2HPA <-> DHPA                                 | flavin-binding family monooxygenase  |
| R506 | Phenylalanine metabolism                            | 1.2.1.39                             | ABAYE1712   | PACAL + NAD <-> PLA + NADH                    | phenylacetaldehyde dehydrogenase   |
| R507 | Phenylalanine metabolism                            | 1.4.3.21                             | ABAYE1710   | PEA + O2 <-> PACAL + NH3 + H2O2               | copper amine oxidase precursor (tyramine oxidase) (2-phenylethylamine oxidase)   |
| R508 | Phenylalanine metabolism                            | 2.3.1.-                              | ABAYE0497 OR<br>ABAYE0625 OR<br>ABAYE1513 OR<br>ABAYE1675 OR<br>ABAYE1715 OR<br>ABAYE1811 OR<br>ABAYE2153 OR<br>ABAYE2367 OR<br>ABAYE2457 OR<br>ABAYE2483 OR<br>ABAYE3572 OR<br>ABAYE3588 OR<br>ABAYE3697 OR<br>ABAYE3807 | PACOA + GLY <-> PACGLY + COA                  | acyltransferase OR acetyl transferase OR acyl-CoA thiolase OR beta-ketoacyl CoA thiolase OR GCN5-related N-acetyltransferase |
| R509 | Phenylalanine metabolism                            | 3.5.1.32                             | ABAYE3086   | HIPPRT <-> BZ + GLY                           | hydrolase  |
| R510 | Phenylalanine metabolism                            | 3.5.1.4                              | ABAYE1700 OR<br>ABAYE2422   | PAA <-> PLA + NH3                             | amidase  |
| R511 | Phenylalanine metabolism                            | 6.2.1.30                             | ABAYE2366   | ATP + PLA + COA <-> AMP + PPI + PACOA         | phenylacetate-coenzyme A ligase (phenylacetyl-CoA ligase)  |
| R512 | Tryptophan metabolism                               | 6.1.1.2                              | ABAYE0788   | ATP + TRP + TRNATRP -> AMP + PPI + TRPTRNATRP | tryptophanyl-tRNA synthetase   |
| R513 | Tryptophan metabolism                               | 1.2.1.3                              | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | 5HIAA + NAD -> 5HIAC + NADH                   | aldehyde dehydrogenase   |
| R514 | Tryptophan metabolism                               | 1.2.1.3                              | ABAYE1028 OR<br>ABAYE1460 OR<br>ABAYE2333 OR<br>ABAYE2837   | I3AA + NAD -> I3AC + NADH                     | aldehyde dehydrogenase   |
| R515 | Tryptophan metabolism                               | 1.11.1.6                             | ABAYE2270 OR<br>ABAYE2342 OR<br>ABAYE3366   | 2 3HAN + 2 O2 -> CVN + 2 H2O2                 | catalase   |
| R516 | Tryptophan metabolism                               | 1.2.4.2                              | ABAYE0780   | 2OAD + COA + NAD -> GLUTCOA + CO2 + NADH      | 2-oxoglutarate dehydrogenase E1 component  |
| R517 | Tryptophan metabolism                               | 2.1.1.-                              | ABAYE0624 OR<br>ABAYE2481 OR<br>ABAYE2566 OR<br>ABAYE2771 OR<br>ABAYE2871   | AEIOH + MTHF <-> MOT + THF                    | methyltransferase  |
| R518 | Tryptophan metabolism                               | 3.5.1.4                              | ABAYE1700 OR<br>ABAYE2422   | I3AAM <-> I3AC + NH3                          | amidase  |
| R519 | Tryptophan metabolism                               | 3.7.1.3                              | ABAYE1599   | FKYN <-> FAN + ALA                            | L-tryptophan hydroxylase   |
| R520 | Tryptophan metabolism                               | 3.7.1.3                              | ABAYE1599   | KYN <-> AN + ALA                              | L-tryptophan hydroxylase   |
| R521 | Tryptophan metabolism                               | 3.7.1.3                              | ABAYE1599   | HKYN <-> 3HAN + ALA                           | L-tryptophan hydroxylase   |
| R522 | Tryptophan metabolism                               | 4.1.1.74                             | ABAYE1030   | IPYR <-> I3AA + CO2                           | pyruvate decarboxylase OR indolepyruvate decarboxylase   |
| R523 | Phenylalanine, tyrosine and tryptophan biosynthesis | 2.5.1.54                             | ABAYE1658 OR<br>ABAYE1989   | E4P + PEP -> PI + 3DDAH7P                     | 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase   |
| R524 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.3.4                              | ABAYE0296   | 3DDAH7P -> DQT + PI                           | 3-dehydroquinate synthetase  |
| R525 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.1.10                             | ABAYE1539 OR<br>ABAYE1682   | DQT <-> DHSK                                  | 3-dehydroquinate dehydratase II OR catabolic 3-dehydroquinate dehydratase (3-dehydroquinase)                                 |
| R526 | Phenylalanine, tyrosine and tryptophan biosynthesis | 1.1.1.25                             | ABAYE0377   | DHSK + NADPH -> SME + NADP                    | shikimate 5-dehydrogenase  |
| R527 | Phenylalanine, tyrosine and tryptophan biosynthesis | 2.7.1.71                             | ABAYE0295   | SME + ATP -> ADP + SME3P                      | shikimate kinase   |
| R528 | Phenylalanine, tyrosine and tryptophan biosynthesis | 2.5.1.19                             | ABAYE1207   | SME3P + PEP -> 3PSME + PI                     | 3-phosphoshikimate 1-carboxyvinyltransferase   |
| R529 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.3.5                              | ABAYE1953   | 3PSME -> PI + CHOR                            | chorismate synthase  |
| R530 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.1.3.27                             | ABAYE1123 OR<br>ABAYE3497   | CHOR + GLN -> GLU + PYR + AN                  | anthranilate synthase  |
| R531 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.1.3.27                             | ABAYE1123 OR<br>ABAYE3497   | CHOR + NH3 -> AN + PYR                        | anthranilate synthase  |
| R532 | Phenylalanine, tyrosine and tryptophan biosynthesis | 2.4.2.18                             | ABAYE1119   | AN + PRPP -> PPI + NPRAN                      | anthranilate phosphoribosyltransferase   |
| R533 | Phenylalanine, tyrosine and tryptophan biosynthesis | 5.3.1.24                             | ABAYE0607   | NPRAN -> CPAD5P                               | phosphoribosylanthranilate isomerase   |
| R534 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.1.1.48                             | ABAYE1118   | CPAD5P -> CO2 + IGP                           | indole-3-glycerol phosphate synthase   |
| R535 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.1.20                             | ABAYE0608 OR<br>ABAYE0613 OR<br>ABAYE1955   | IGP + SER -> G3P + TRP                        | tryptophan synthase  |
| R536 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.1.20                             | ABAYE0608 OR<br>ABAYE1955   | SER + INDOLE -> TRP                           | tryptophan synthase  |
| R537 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.1.20                             | ABAYE0613   | INDOLE + G3P <-> IGP                          | tryptophan synthase  |
| R538 | Phenylalanine, tyrosine and tryptophan biosynthesis | 5.4.99.5                             | ABAYE1206 OR<br>ABAYE1477   | CHOR <-> PHEN                                 | chorismate mutase  |
| R539 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.1.51                             | ABAYE1206   | PHEN -> CO2 + PHPYR                           | prephenate dehydratase   |
| R540 | Phenylalanine, tyrosine and tryptophan biosynthesis | 6.1.1.20                             | ABAYE3159 AND<br>ABAYE3160  | ATP + PHE + TRNAPHE -> AMP + PPI + PHETRNAPHE | phenylalanyl-tRNA synthetase   |
| R541 | Phenylalanine, tyrosine and tryptophan biosynthesis | 1.3.1.12                             | ABAYE1207   | PHEN + NAD -> 4HPP + CO2 + NADH               | prephenate dehydrogenase   |
| R542 | Phenylalanine, tyrosine and tryptophan biosynthesis | 2.6.1.1 OR<br>2.6.1.9 OR<br>2.6.1.57 | ABAYE0951 OR<br>ABAYE3130 OR<br>ABAYE3795   | 4HPP + GLU -> AKG + TYR                       | histidinol-phosphate aminotransferase  |



| No.  | Metabolism  | EC Number           | ORF   | Reaction  | Enzyme  |
|------|---|---------------------|---|---|---|
| R543 | Phenylalanine, tyrosine and tryptophan biosynthesis | 6.1.1.1             | ABAYE0014   | ATP + TYR + TRNATYR -> AMP + PPI + TRYTRNATYR   | tyrosyl-tRNA synthetase   |
| R544 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.1.51            | ABAYE1206   | AG -> PHE + CO2                                 | prephenate dehydratase  |
| R545 | Phenylalanine, tyrosine and tryptophan biosynthesis | 1.1.99.25           | ABAYE1685   | QNT + PQQ <-> PQQH2 + DQT                       | quininate/shikimate dehydrogenase   |
| R546 | Phenylalanine, tyrosine and tryptophan biosynthesis | 1.1.99.25           | ABAYE1685   | SME + PQQ <-> DHSK + PQQH2                      | quininate/shikimate dehydrogenase   |
| R547 | Phenylalanine, tyrosine and tryptophan biosynthesis | 4.2.1.- (QuiC)      | ABAYE1683   | DHSK <-> 34DHB                                  | 3-dehydroshikimate dehydratase OR DHS dehydratase   |
| R548 | Urea cycle and metabolism of amino groups           | 2.7.2.11            | ABAYE0962   | GLU + ATP -> ADP + GLUP                         | glutamate 5-kinase  |
| R549 | Urea cycle and metabolism of amino groups           | 1.2.1.41            | ABAYE3276   | GLUP + NADPH -> NADP + PI + GLUGSAL             | gamma-glutamyl phosphate reductase  |
| R550 | Urea cycle and metabolism of amino groups           |                     |   | GLUGSAL <-> P5C                                 | spontaneous   |
| R551 | Urea cycle and metabolism of amino groups           | 1.5.1.2             | ABAYE2533 OR ABAYE3151  | P5C + NADPH <-> PRO + NADP                      | pyrroline-5-carboxylate reductase   |
| R552 | Urea cycle and metabolism of amino groups           | 1.5.1.2             | ABAYE2533 OR ABAYE3151  | PRO + NAD <-> P5C + NADH                        | pyrroline-5-carboxylate reductase   |
| R553 | Urea cycle and metabolism of amino groups           | 2.3.1.1             | ABAYE3105 OR ABAYE3839  | GLU + ACCOA -> COA + NAGLU                      | amino-acid N-acetyltransferase  |
| R554 | Urea cycle and metabolism of amino groups           | 2.7.2.8             | ABAYE2927   | NAGLU + ATP -> ADP + NAGLUP                     | acetylglutamate kinase  |
| R555 | Urea cycle and metabolism of amino groups           | 1.2.1.38            | ABAYE1653   | NAGLUP + NADPH -> NADP + PI + NAGLUS            | N-acetyl-gamma-glutamyl-phosphate reductase   |
| R556 | Urea cycle and metabolism of amino groups           | 2.6.1.11            | ABAYE1625   | NAGLUS + GLU -> AKG + NAORN                     | acetylmornithine aminotransferase   |
| R557 | Urea cycle and metabolism of amino groups           | 2.3.1.35            | ABAYE3105   | NAORN + GLU <-> ORN + NAGLU                     | bifunctional ornithine acetyltransferase/N-acetylglutamate synthase                             |
| R558 | Urea cycle and metabolism of amino groups           | 2.1.3.3             | ABAYE1571   | ORN + CAP <-> CITR + PI                         | ornithine carbamoyltransferase  |
| R559 | Urea cycle and metabolism of amino groups           | 6.3.4.5             | ABAYE2641   | CITR + ASP + ATP <-> AMP + PPI + ARGSUCC        | argininosuccinate synthase  |
| R560 | Urea cycle and metabolism of amino groups           | 4.3.2.1             | ABAYE3511   | ARGSUCC <-> FUM + ARG                           | argininosuccinate lyase   |
| R561 | Urea cycle and metabolism of amino groups           | 1.2.1.3             | ABAYE1028 OR ABAYE1460 OR ABAYE2333 OR ABAYE2837              | N4AAB + NAD <-> 4AABUT + NADH                   | aldehyde dehydrogenase  |
| R562 | Urea cycle and metabolism of amino groups           | 1.2.1.3             | ABAYE1028 OR ABAYE1460 OR ABAYE2333 OR ABAYE2837              | 4AB + NADP <-> GABA + NADPH                     | aldehyde dehydrogenase  |
| R563 | Urea cycle and metabolism of amino groups           | 3.2.2.9             | ABAYE3028 OR ABAYE3846  | 5MTA <-> AD + 5MDR                              | 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase                                      |
| R564 | Urea cycle and metabolism of amino groups           | 3.4.13.3            | ABAYE1209   | HCNS <-> GABA + HIS                             | aminoacyl-histidine dipeptidase   |
| R565 | Urea cycle and metabolism of amino groups           | 3.5.1.4             | ABAYE1700 OR ABAYE2422  | 4GBTA <-> 4GBTR + NH3                           | amidase   |
| R566 | Urea cycle and metabolism of amino groups           | 3.5.1.5             | ABAYE2776 AND ABAYE2777 AND ABAYE2778                         | UREA <-> CO2 + 2 NH3                            | urease  |
| R567 | Urea cycle and metabolism of amino groups           | 3.5.1.54            | ABAYE2439   | U1C <-> 2 CO2 + 2 NH3                           | allophanate hydrolase   |
| R568 | beta-Alanine metabolism                             | 1.2.1.3             | ABAYE1028 OR ABAYE1460 OR ABAYE2333 OR ABAYE2837              | bAPA + NAD -> bALA + NADH                       | aldehyde dehydrogenase (NAD+)   |
| R569 | beta-Alanine metabolism                             | 1.4.3.21            | ABAYE1710   | 13DAP + O2 <-> 3AP + NH3 + H2O2                 | copper amine oxidase precursor (tyramine oxidase) (2-phenylethylamine oxidase)                  |
| R570 | beta-Alanine metabolism                             | 2.6.1.18            | ABAYE1295   | ALA + 3OPP <-> PYR + bALA                       | omega-amino acid-pyruvate aminotransferase (omega-APT) (beta-alanine-pyruvate aminotransferase) |
| R571 | beta-Alanine metabolism                             | 2.6.1.19            | ABAYE0209   | bALA + AKG <-> OPP + GLU                        | 4-aminobutyrate aminotransferase, PLP-dependent   |
| R572 | beta-Alanine metabolism                             | 4.1.1.11            | ABAYE2984   | ASP -> bALA + CO2                               | aspartate 1-decarboxylase precursor   |
| R573 | Taurine and hypotaurine metabolism                  | 1.14.11.17          | ABAYE2209   | TR + AKG + O2 -> H2SO3 + AAA + SUCC + CO2       | taurine dioxygenase   |
| R574 | Taurine and hypotaurine metabolism                  | 2.3.2.2             | ABAYE2905   | 5GLUPEPT + TR -> PEPTIDE + GLUTR                | gamma-glutamyltranspeptidase precursor  |
| R575 | Aminophosphonate metabolism                         | 2.6.1.37            | ABAYE2318   | (2AE)P + PYR <-> PPAC + ALA                     | 2-aminoethylphosphonate-pyruvate transaminase   |
| R576 | Aminophosphonate metabolism                         | 2.1.1.-             | ABAYE0624 OR ABAYE2481 OR ABAYE2566 OR ABAYE2771 OR ABAYE2871 | MCB + PPAC -> 2HPP + VB12                       | N6-adenine-specific methylase   |
| R577 | Aminophosphonate metabolism                         | 2.7.8.-             | ABAYE1103 OR ABAYE3258 OR ABAYE3750                           | CMPAEP + NAS <-> NASAEP + CMP                   | 4'-phosphopantetheinyl transferase  |
| R578 | Aminophosphonate metabolism                         | 3.11.1.1            | ABAYE2317   | PPAC <-> ACAL + PI                              | phosphonoacetaldehyde phosphonohydrolase (phosphonatase)  |
| R579 | Selenoamino acid metabolism                         | 4.4.1.8             | ABAYE0405   | SLLCT -> SHCYS + NH3 + PYR                      | cystathionine beta-lyase  |
| R580 | Selenoamino acid metabolism                         |                     |   | SHCYS -> SMET                                   |   |
| R581 | Selenoamino acid metabolism                         | 6.1.1.10            | ABAYE3031   | ATP + SMET + TRNAMET -> AMP + PPI + SMETTRNAMET | methionyl-tRNA synthetase   |
| R582 | Selenoamino acid metabolism                         | 2.5.1.6             | ABAYE2118   | ATP + SMET -> PI + PPI + SeASMET                | S-adenosylmethionine synthetase   |
| R583 | Selenoamino acid metabolism                         | 2.5.1.47            | ABAYE3184 OR ABAYE3696  | ASER + SELD -> SCYS + AC                        | cysteine synthase   |
| R584 | Selenoamino acid metabolism                         | 2.7.7.4             | ABAYE2790 AND ABAYE2791                                       | ATP + SELNT <-> PPI + ASELNT                    | sulfate adenyltransferase   |
| R585 | Selenoamino acid metabolism                         | 2.3.2.2             | ABAYE2905   | 5GLUPEPT + MSCYS -> PEPTIDE + GGLUMSCYS         | gamma-glutamyltranspeptidase precursor  |
| R586 | Selenoamino acid metabolism                         | 3.3.1.1             | ABAYE1142   | SASHCYS <-> ADN + SHCYS                         | S-adenosyl-L-homocysteine hydrolase   |
| R587 | Selenoamino acid metabolism                         | 4.4.1.16            | ABAYE2250   | SCYS + FADH2 <-> SELD + ALA + FAD               | cysteine desulfurase 1 OR selenocysteine lyase  |
| R588 | Cyanoamino acid metabolism                          | 2.3.2.2             | ABAYE2905   | CALA + GLU -> GLUBCALA                          | gamma-glutamyltranspeptidase precursor  |
| R589 | Cyanoamino acid metabolism                          | 2.3.2.2             | ABAYE2905   | APN + GLU -> GAPN                               | gamma-glutamyltranspeptidase precursor  |
| R590 | D-Glutamine and D-glutamate metabolism              | 3.5.1.2 OR 3.5.1.38 | ABAYE2832 OR ABAYE2188  | DGLN -> DGLU + NH3                              | glutaminase OR glutaminase-asparaginase   |
| R591 | D-Glutamine and D-glutamate metabolism              | 5.1.1.3             | ABAYE0082 OR ABAYE3395  | DGLU <-> GLU                                    | glutamate racemase  |
| R592 | D-Alanine metabolism                                | 5.1.1.1             | ABAYE1380 OR ABAYE3773  | ALA <-> DALA                                    | alanine racemase  |
| R593 | D-Alanine metabolism                                | 6.3.2.4             | ABAYE0150   | 2 DALA + ATP -> ALAALA + ADP + PI               | D-alanine-D-alanine ligase  |

| No.  | Metabolism                                | EC Number                              | ORF                                       | Reaction  | Enzyme  |
|------|---|--|---|---|---|
| R594 | Glutathione metabolism                    | 3.4.11.1 OR<br>3.4.11.2 OR<br>3.4.13.3 | ABAYE3540 OR<br>ABAYE1469 OR<br>ABAYE1209 | CYSGLY -> CYS + GLY   | aminopeptidase A (EC:3.4.11.1) OR membrane<br>alanyl aminopeptidase OR aminoacyl-histidine<br>dipeptidase (peptidase D) (EC:3.4.13.3) |
| R595 | Glutathione metabolism                    | 1.11.1.9                               | ABAYE2184 OR<br>ABAYE3713                 | H2O2 + 2 RGT <=> OGT  | glutathione peroxidase  |
| R596 | Glutathione metabolism                    | 2.3.2.2                                | ABAYE2905                                 | RGT -> CYSGLY + GLU   | gamma-glutamyltranspeptidase precursor  |
| R597 | Glutathione metabolism                    | 6.3.2.2                                | ABAYE0116                                 | ATP + GLU + CYS <=> ADP + PI + GCYS                                   | gamma-glutamyl-cysteine ligase  |
| R598 | Glutathione metabolism                    | 6.3.2.3                                | ABAYE0147                                 | ATP + GCYS + GLY <=> ADP + PI + RGT                                   | glutathione synthetase  |
| R599 | Lipopolysaccharide biosynthesis           | 2.3.1.129                              | ABAYE1587                                 | C140ACP + UDPNAG -> ACP + UDPG2AA                                     | UDP-N-acetylglucosamine acyltransferase   |
| R600 | Lipopolysaccharide biosynthesis           | 3.5.1.-                                | ABAYE0154                                 | UDPG2AA -> UDPG2A + AC  | UDP-3-O-[3-hydroxy-myristoyl]-N-<br>acetylglucosamine deacetylase   |
| R601 | Lipopolysaccharide biosynthesis           | 2.3.1.-                                | ABAYE1585                                 | UDPG2A + C140ACP -> ACP + UDPG23A                                     | UDP-3-O-[3-hydroxy-myristoyl] glucosamine<br>N-acyltransferase  |
| R602 | Lipopolysaccharide biosynthesis           | 3.6.1.-                                | ABAYE1453                                 | UDPG23A -> UMP + LIPX   | UDP-2,3-diacetylglucosamine hydrolase   |
| R603 | Lipopolysaccharide biosynthesis           | 2.4.1.182                              | ABAYE1983                                 | LIPX + UDPG23A -> UDP + DISAC1P                                       | lipid-A-disaccharide synthase   |
| R604 | Lipopolysaccharide biosynthesis           | 2.7.1.130                              | ABAYE2077                                 | DISAC1P + ATP -> ADP + LIPIV  | tetraacyldisaccharide 4'-kinase   |
| R605 | Lipopolysaccharide biosynthesis           | 2.-.-.-                                | ABAYE0175                                 | LIPIV + CMPKDO -> KDOLIPIV + CMP                                      | 3-deoxy-D-manno-octulosonic-acid transferase  |
| R606 | Lipopolysaccharide biosynthesis           | 2.-.-.-                                | ABAYE0175                                 | KDOLIPIV + CMPKDO -> K2LIPIV + CMP                                    | 3-deoxy-D-manno-octulosonic-acid transferase  |
| R607 | Lipopolysaccharide biosynthesis           | 2.3.1.-                                | ABAYE0885 OR<br>ABAYE3343                 | C140ACP + LK2LIPIV -> K2LIPA + ACP                                    | lipid A biosynthesis (KDO)2-(lauroyl)-lipid iv<br>acyltransferase   |
| R608 | Lipopolysaccharide biosynthesis           | 5.3.1.13                               |   | RL5P <=> A5P  | D-arabinose 5-phosphate isomerase   |
| R609 | Lipopolysaccharide biosynthesis           | 2.5.1.55                               | ABAYE1668                                 | PEP + A5P -> KDOP + PI  | 2-dehydro-3-deoxyphosphoactonate aldolase<br>(KDO 8-P synthase)   |
| R610 | Lipopolysaccharide biosynthesis           | 3.1.3.45                               | ABAYE2491                                 | KDOP -> KDO + PI  | 3-deoxy-D-manno-octulosonate 8-phosphate<br>phosphatase   |
| R611 | Lipopolysaccharide biosynthesis           | 2.7.7.38                               | ABAYE2076                                 | KDO + CTP -> PPI + CMPKDO   | 3-deoxy-manno-octulosonate cytidyltransferase   |
| R612 | Peptidoglycan biosynthesis                | 6.3.2.8                                | ABAYE0149                                 | UDPNAM + ALA + ATP -> ADP + PI + UDPNAMA                              | UDP-N-acetylmuramate-alanine ligase   |
| R613 | Peptidoglycan biosynthesis                | 6.3.2.9                                | ABAYE3524                                 | UDPNAMA + DGLU + ATP -> UDPNAMAG + ADP +<br>PI                        | UDP-N-acetylmuramoylalanine--D-glutamate<br>ligase  |
| R614 | Peptidoglycan biosynthesis                | 6.3.2.13                               | ABAYE0283                                 | UDPNAMAG + MDAPIM + ATP -> UDPMNLADGMD<br>+ ADP + PI                  | UDP-N-acetylmuramoylalanine-D-glutamate--2,6-<br>diaminopimelate ligase   |
| R615 | Peptidoglycan biosynthesis                | 6.3.2.10                               | ABAYE0284                                 | UDPMNLADGMD + ALAALA + ATP -><br>UDPMNLADGMDDADA + ADP + PI           | UDP-N-acetylmuramoyl-tripeptide--D-alanyl-D-<br>alanine ligase  |
| R616 | Peptidoglycan biosynthesis                | 2.7.8.13                               | ABAYE0285                                 | UDPMNLADGMDDADA + UDCP -><br>UPPMNLADGMDDADA + UMP                    | phospho-N-acetylmuramoyl-pentapeptide-<br>transferase   |
| R617 | Peptidoglycan biosynthesis                | 2.4.1.227                              | ABAYE0148                                 | UPPMNLADGMDDADA + UDPNAG -><br>UPPMN(GN)LADGMDDADA + UDP              | UDP-N-acetylglucosamine--N acetylmuramyl-<br>(pentapeptide)<br>pyrophosphoryl-undecaprenol N-<br>acetylglucosamine transferase        |
| R618 | Peptidoglycan biosynthesis                | 6.3.1.2                                | ABAYE1126 OR<br>ABAYE1425                 | UPPMN(GN)LADGMDDADA + ATP + NH3 -><br>UPPMN(GN)LADGNMDDADA + ADP + PI | glutamine synthetase  |
| R619 | Peptidoglycan biosynthesis                | 2.3.2.10                               |   | 5 GLY + UPPMN(GN)LADGNMDDADA -><br>UPPMN(GN)LADGNMD(G)5DADA           | L-Alanyl-tRNA:UDP-N-acetylmuramoyl-L-alanyl-D-<br>glutamyl-L-lysyl-D-<br>alanyl-D-alanine N6-alanyltransferase                        |
| R620 | Peptidoglycan biosynthesis                |  |   | UPPMN(GN)LADGNMD(G)5DADA -> UDCPP +<br>PPEPTIDO                       |   |
| R621 | Peptidoglycan biosynthesis                | 2.6.1.21                               |   | PPEPTIDO + DALA -> 0.9208 PEPTIDO + 0.8<br>DALAx                      | D-Alanine:2-oxoglutarate aminotransferase   |
| R622 | Peptidoglycan biosynthesis                | 3.6.1.27                               | ABAYE0716                                 | UDCPP -> UDCP + PI  | undecaprenyl-diphosphatase  |
| R623 | Thiamine metabolism                       | thiC                                   | ABAYE3518                                 | AIR -> AHM  | thiamine biosynthesis protein ThiC  |
| R624 | Thiamine metabolism                       | 2.7.1.49                               | ABAYE2989                                 | AHM + ATP -> AHMP + ADP   | hydroxymethylpyrimidine kinase  |
| R625 | Thiamine metabolism                       | 2.7.4.7                                | ABAYE2989                                 | AHMP + ATP -> AHMPP + ADP   | phosphomethylpyrimidine kinase  |
| R626 | Thiamine metabolism                       | 2.5.1.3                                | ABAYE1010                                 | TH2P + AHMPP -> THMP + PPI  | thiamine-phosphate pyrophosphorylase  |
| R627 | Thiamine metabolism                       | 2.7.4.16                               | ABAYE0093                                 | THMP + ATP <=> THMPP + ADP  | thiamine-monophosphate kinase   |
| R628 | Thiamine metabolism                       | 1.4.3.19                               | ABAYE2910                                 | GLY <=> IGLY  | D-amino acid oxidase  |
| R629 | Thiamine metabolism                       | 2.7.1.50                               | ABAYE1466                                 | ATP + THZ <=> ADP + MPET  | hydroxyethylthiazole kinase   |
| R630 | Thiamine metabolism                       | 3.5.99.2                               | ABAYE0200                                 | THIAMIN <=> AHM + THZ   | TenA family transcriptional activator   |
| R631 | Thiamine metabolism                       | 3.6.1.15                               | ABAYE3296                                 | THMPP <=> THMP + PI   | nucleoside-triphosphatase   |
| R632 | Riboflavin metabolism                     | 3.5.4.25                               | ABAYE0096 OR<br>ABAYE0379                 | GTP -> D6RP5P + FORMATE + PPI   | GTP cyclohydrolase II   |
| R633 | Riboflavin metabolism                     | 3.5.4.26                               | ABAYE3546                                 | D6RP5P -> A6RP5P + NH3  | diaminohydroxyphosphoribosylaminopyrimidine<br>deaminase  |
| R634 | Riboflavin metabolism                     | 1.1.1.193                              | ABAYE3546                                 | A6RP5P + NADPH -> A6RP5P2 + NADP                                      | 5-amino-6-(5-phosphoribosylamino)uracil<br>reductase  |
| R635 | Riboflavin metabolism                     | 3.1.3.-                                |   | A6RP5P2 -> A6RP + PI  | phosphatase   |
| R636 | Riboflavin metabolism                     | RIBB                                   | ABAYE0096 OR<br>ABAYE2987                 | RL5P -> DB4P + FORMATE  | 3,4-dihydroxy-2-butanone 4-phosphate synthase   |
| R637 | Riboflavin metabolism                     | RIBH                                   | ABAYE0095                                 | DB4P + A6RP -> D8RL + PI  | riboflavin synthase   |
| R638 | Riboflavin metabolism                     | 2.5.1.9                                | ABAYE3544                                 | 2 D8RL -> RIBFLAV + A6RP  | riboflavin synthase   |
| R639 | Riboflavin metabolism                     | 2.7.1.26                               | ABAYE3851                                 | RIBFLAV + ATP -> FMN + ADP  | riboflavin kinase   |
| R640 | Riboflavin metabolism                     | 2.7.7.2                                | ABAYE3851                                 | FMN + ATP -> FAD + PPI  | FMN adenylyltransferase   |
| R641 | Riboflavin metabolism                     | 2.4.2.21                               | ABAYE1993                                 | NACN + DMB -> NAC + N1(5PADR)DMB                                      | nicotinate-nucleotide--dimethylbenzimidazole<br>phosphoribosyltransferase   |
| R642 | Vitamin B6 metabolism                     | 1.2.1.72                               | ABAYE2594                                 | E4P + NAD <=> ER4P + NADH   | D-erythrose 4-phosphate dehydrogenase   |
| R643 | Vitamin B6 metabolism                     | 1.1.1.290                              | ABAYE0853                                 | ER4P + NAD <=> OHB + NADH   | erythronate-4-phosphate dehydrogenase   |
| R644 | Vitamin B6 metabolism                     | 2.6.1.52                               | ABAYE0877                                 | OHB + GLU <=> PHT + AKG   | phosphoserine aminotransferase  |
| R645 | Vitamin B6 metabolism                     | 4.2.3.1                                | ABAYE3531                                 | PHT -> 4HLT + PI  | threonine synthase  |
| R646 | Vitamin B6 metabolism                     | 1.1.1.262                              | ABAYE0489                                 | PHT + NAD -> 3A2OP + NADH + CO2                                       | 4-hydroxythreonine-4-phosphate dehydrogenase  |
| R647 | Vitamin B6 metabolism                     | 2.6.99.2                               | ABAYE0945                                 | 3A2OP + DX5P -> P5P + PI  | pyridoxine 5-phosphate synthase   |
| R648 | Vitamin B6 metabolism                     | 1.4.3.5                                | ABAYE0168                                 | P5P + O2 -> PL5P + H2O2   | pyridoxamine 5'-phosphate oxidase   |
| R649 | Vitamin B6 metabolism                     | 3.1.3.-                                |   | PL5P -> PL + PI   | phosphatase   |
| R650 | Vitamin B6 metabolism                     | 1.4.3.5                                | ABAYE0168                                 | PDLA5P + O2 -> PL5P + NH3 + H2O2                                      | pyridoxamine 5'-phosphate oxidase   |
| R651 | Vitamin B6 metabolism                     | 1.4.3.5                                | ABAYE0168                                 | PYRDX + O2 <=> PL + H2O2  | pyridoxamine 5'-phosphate oxidase   |
| R652 | Vitamin B6 metabolism                     | 1.4.3.5                                | ABAYE0168                                 | PL + O2 + NH3 <=> PDLA + H2O2   | pyridoxamine 5'-phosphate oxidase   |
| R653 | Nicotinate and nicotinamide<br>metabolism | 1.4.3.16                               | ABAYE0935                                 | ASP + FUM -> IASP + SUCC  | L-aspartate oxidase   |
| R654 | Nicotinate and nicotinamide<br>metabolism | 1.4.3.16                               | ABAYE0935                                 | ASP + O2 -> IASP + H2O2   | L-aspartate oxidase   |
| R655 | Nicotinate and nicotinamide<br>metabolism | NadA                                   | ABAYE3104                                 | IASP + DHAP -> QA + PI  | quinolinate synthase  |
| R656 | Nicotinate and nicotinamide<br>metabolism | 2.4.2.19                               | ABAYE3823                                 | QA + PRPP -> NACN + CO2 + PPI   | nicotinate-nucleotide pyrophosphorylase<br>(carboxylating)  |
| R657 | Nicotinate and nicotinamide<br>metabolism | 3.1.3.5                                | ABAYE1047 OR<br>ABAYE1886                 | NACN -> NACD + PI   | 5'-nucleotidase   |
| R658 | Nicotinate and nicotinamide<br>metabolism | 3.1.3.5                                | ABAYE1047 OR<br>ABAYE1886                 | NAMN -> NAMD + PI   | 5'-nucleotidase   |
| R659 | Nicotinate and nicotinamide<br>metabolism | 2.4.2.11                               | ABAYE0102                                 | NAC + PRPP -> NACN + PPI  | nicotinate phosphoribosyltransferase  |
| R660 | Nicotinate and nicotinamide<br>metabolism | 2.7.7.1 OR<br>2.7.7.18                 | ABAYE0916 OR<br>ABAYE0916                 | ATP + NAMN <=> PPI + NAD  | nicotinamide/nicotinate-nucleotide<br>adenylyltransferase   |
| R661 | Nicotinate and nicotinamide<br>metabolism | 2.7.7.1 OR<br>2.7.7.18                 | ABAYE0916 OR<br>ABAYE0916                 | NACN + ATP -> PPI + NAAD  | nicotinate-nucleotide adenylyltransferase   |
| R662 | Nicotinate and nicotinamide<br>metabolism | 6.3.5.1                                | ABAYE2955                                 | NAAD + ATP + GLN -> NAD + AMP + PPI + GLU                             | glutamine-dependent NAD(+) synthetase   |

| No.  | Metabolism                             | EC Number            | ORF  | Reaction                                  | Enzyme   |
|------|--|----------------------|--|---|--|
| R663 | Nicotinate and nicotinamide metabolism | 3.5.1.19             | ABAYE0059  | NAM -> NAC + NH3                          | nicotinamidase   |
| R664 | Nicotinate and nicotinamide metabolism | 1.6.1.2              | ABAYE3191 AND ABAYE3192 AND ABAYE3193            | NADP + NADH -> NADPH + NAD                | NAD(P) transhydrogenase  |
| R665 | Nicotinate and nicotinamide metabolism | 2.7.1.23             | ABAYE1199  | NAD + ATP -> NADP + ADP                   | NAD kinase   |
| R666 | Nicotinate and nicotinamide metabolism | 1.6.1.1              | ABAYE1147  | NADPH + NAD <-> NADP + NADH               | NAD(P) transhydrogenase  |
| R667 | Nicotinate and nicotinamide metabolism | 1.4.1.21             | ABAYE2838  | ASP + NAD <-> IASP + NADH                 | L-aspartate dehydrogenase  |
| R668 | Nicotinate and nicotinamide metabolism | 1.4.1.21             | ABAYE2838  | ASP + NADP <-> IASP + NADPH               | L-aspartate dehydrogenase  |
| R669 | Nicotinate and nicotinamide metabolism | 3.6.1.22             | ABAYE2666  | NAD <-> AMP + NAMN                        | NUDIX family NADH pyrophosphatase  |
| R670 | Nicotinate and nicotinamide metabolism | 3.6.1.22             | ABAYE2666  | NAAD <-> AMP + NACN                       | NUDIX family NADH pyrophosphatase  |
| R671 | Pantothenate and CoA biosynthesis      | 2.2.1.6              | ABAYE2836 OR (ABAYE3239 AND ABAYE3240)           | 2 PYR -> ACLAC + CO2                      | acetolactate synthase  |
| R672 | Pantothenate and CoA biosynthesis      | 2.1.2.11             | ABAYE3175  | OIVAL + METTHF -> DHPANT + THF            | 3-methyl-2-oxobutanoate hydroxymethyltransferase   |
| R673 | Pantothenate and CoA biosynthesis      | 1.1.1.169            |  | DHPANT + NADPH -> NADP + PANT             | 2-dehydropantoate 2-reductase  |
| R674 | Pantothenate and CoA biosynthesis      | 6.3.2.1              | ABAYE3174  | PANT + bALA + ATP -> AMP + PPI + PNT0     | pantoate-beta-alanine ligase   |
| R675 | Pantothenate and CoA biosynthesis      | 2.7.1.33             | ABAYE3016  | PNT0 + ATP -> ADP + 4PPNT0                | pantothenate kinase  |
| R676 | Pantothenate and CoA biosynthesis      | 2.7.1.33             | ABAYE3016  | ATP + N(P)CYS -> ADP + 4PPNCYS            | pantothenate kinase  |
| R677 | Pantothenate and CoA biosynthesis      | 2.7.1.33             | ABAYE3016  | ATP + PTT -> ADP + 4PPNTE                 | pantothenate kinase  |
| R678 | Pantothenate and CoA biosynthesis      | 6.3.2.5              | ABAYE0524  | 4PPNT0 + CTP + CYS -> CMP + PPI + 4PPNCYS | phosphopantothenate-cysteine ligase  |
| R679 | Pantothenate and CoA biosynthesis      | 4.1.1.36             | ABAYE0524  | 4PPNCYS -> CO2 + 4PPNTE                   | phosphopantothenoylecysteine decarboxylase   |
| R680 | Pantothenate and CoA biosynthesis      | 2.7.7.3              | ABAYE2969  | 4PPNTE + ATP -> PPI + DPCOA               | pantetheine-phosphate adenyltransferase  |
| R681 | Pantothenate and CoA biosynthesis      | 2.7.1.24             | ABAYE3447  | DPCOA + ATP -> ADP + COA                  | dephospho-CoA kinase   |
| R682 | Biotin metabolism                      | 2.3.1.47             | ABAYE3003  | ALA + CHCOA <-> CO2 + COA + AONA          | 8-amino-7-oxononanoate synthase  |
| R683 | Biotin metabolism                      | 2.6.1.62             | ABAYE3004  | SAM + AONA <-> SAMOB + DANNA              | adenosylmethionine-8-amino-7-oxononanoateaminotransferase  |
| R684 | Biotin metabolism                      | 6.3.3.3              | ABAYE3001  | CO2 + DANNA + ATP <-> DTB + PI + ADP      | dethiobiotin synthetase  |
| R685 | Biotin metabolism                      | 2.8.1.6              | ABAYE2129  | DTB + S -> BT                             | biotin synthase  |
| R686 | Biotin metabolism                      | 6.3.4.15             | ABAYE3015  | ATP + BT -> PPI + B5AMP                   | biotin-[acetyl-CoA-carboxylase] ligase   |
| R687 | Biotin metabolism                      | 6.3.4.15             | ABAYE3015  | B5AMP + A[C] -> AMP + H[C]                | biotin-[acetyl-CoA-carboxylase] ligase   |
| R688 | Folate biosynthesis                    | 3.5.4.16             | ABAYE1113  | GTP -> FORMATE + AHTD                     | GTP cyclohydrolase I   |
| R689 | Folate biosynthesis                    | 3.6.1.-              | ABAYE3429  | AHTD -> DHP + PPI + PI                    | recG-like helicase   |
| R690 | Folate biosynthesis                    | 4.1.2.25             | ABAYE1417  | DHP -> AHHMP + GLAL                       | dihydroneopterin aldolase  |
| R691 | Folate biosynthesis                    | 2.7.6.3              | ABAYE1418 OR ABAYE3176                           | AHHMP + ATP -> AMP + AHHMD                | 2-amino-4-hydroxy-6-hydroxymethyl-dihydropteridine pyrophosphokinase   |
| R692 | Folate biosynthesis                    | 2.6.1.85             | ABAYE3129  | CHOR + GLN -> ADCHOR + GLU                | para-aminobenzoate synthase  |
| R693 | Folate biosynthesis                    | 4.1.3.38             | ABAYE0931  | ADCHOR -> PYR + PABA                      | 4-amino-4-deoxychorismate lyase  |
| R694 | Folate biosynthesis                    | 2.5.1.15             | ABAYE0807 OR ABAYE3568 OR ABAYE3612 OR ABAYE3616 | PABA + AHHMD -> PPI + DHPT                | dihydropteroate synthase   |
| R695 | Folate biosynthesis                    | 2.5.1.15             | ABAYE0807 OR ABAYE3568 OR ABAYE3612 OR ABAYE3616 | PABA + AHHMP -> DHPT                      | dihydropteroate synthase   |
| R696 | Folate biosynthesis                    | 6.3.2.12 OR 6.3.2.17 | ABAYE0615  | DHPT + ATP + GLU -> ADP + PI + DHF        | dihydrofolate synthase   |
| R697 | Folate biosynthesis                    | 1.5.1.3              | ABAYE3315 OR ABAYE3614 OR ABAYE3644              | DHF + NADPH -> NADP + THF                 | dihydrofolate reductase  |
| R698 | Folate biosynthesis                    | 1.5.1.3              | ABAYE3315 OR ABAYE3614 OR ABAYE3644              | DHF + NADH -> NAD + THF                   | dihydrofolate reductase  |
| R699 | Folate biosynthesis                    | 1.5.1.3              | ABAYE3315 OR ABAYE3614 OR ABAYE3644              | DHF + NAD <-> FL + NADH                   | dihydrofolate reductase  |
| R700 | Folate biosynthesis                    | 1.5.1.3              | ABAYE3315 OR ABAYE3614 OR ABAYE3644              | DHF + NADP <-> FL + NADPH                 | dihydrofolate reductase  |
| R701 | Folate biosynthesis                    | 1.5.1.3              | ABAYE3315 OR ABAYE3614 OR ABAYE3644              | FL + NADH -> THF + NAD                    | dihydrofolate reductase  |
| R702 | Folate biosynthesis                    | 1.5.1.3              | ABAYE3315 OR ABAYE3614 OR ABAYE3644              | FL + NADPH -> THF + NADP                  | dihydrofolate reductase  |
| R703 | Folate biosynthesis                    | 6.3.2.17             | ABAYE0615  | THF + ATP + GLU <-> ADP + PI + THFG       | folylpolyglutamate synthase  |
| R704 | Folate biosynthesis                    | 4.2.3.12             | ABAYE2067  | AHTD -> PYTHP + PPPI                      | 6-pyruvoyl tetrahydropterin synthase   |
| R705 | Folate biosynthesis                    | 3.1.3.1              | ABAYE0811  | AHTD <-> DHP + 3 PI                       | alkaline phosphatase D precursor   |
| R706 | One carbon pool by folate              | 2.1.2.2              | ABAYE0888 OR ABAYE2179                           | GAR + METHF -> FGAR + THF                 | phosphoribosylglycinamide formyltransferase  |
| R707 | One carbon pool by folate              | 3.5.4.9              | ABAYE0812  | METHF -> FTHF                             | bifunctional protein [includes: 5,10-methylene-tetrahydrofolate dehydrogenase; 5,10-methylene-tetrahydrofolate cyclohydrolase] |
| R708 | One carbon pool by folate              | 1.5.1.5              | ABAYE0812  | METTHF + NADP <-> METHF + NADPH           | bifunctional protein [includes: 5,10-methylene-tetrahydrofolate dehydrogenase; 5,10-methylene-tetrahydrofolate cyclohydrolase] |
| R709 | One carbon pool by folate              | 3.5.4.9              | ABAYE0812  | METHF <-> FTHF                            | bifunctional protein [includes: 5,10-methylene-tetrahydrofolate dehydrogenase; 5,10-methylene-tetrahydrofolate cyclohydrolase] |
| R710 | One carbon pool by folate              | 1.5.1.20             | ABAYE1141 OR ABAYE1792                           | METTHF + NADPH -> MTHF + NADP             | methylenetetrahydrofolate reductase  |
| R711 | One carbon pool by folate              | 1.5.1.20             | ABAYE1141 OR ABAYE1792                           | METTHF + FADH2 <-> MTHF + FAD             | methylenetetrahydrofolate reductase  |

| No.  | Metabolism                           | EC Number | ORF                                       | Reaction   | Enzyme   |
|------|--------------------------------------|-----------|---|--|--|
| R712 | One carbon pool by folate            | 2.1.1.45  | ABAYE3314                                 | DUMP + METTHF <-> DHF + DTMP   | thymidylate synthase   |
| R713 | One carbon pool by folate            | 3.5.1.10  | ABAYE3322                                 | FTHF <-> FORMATE + THF   | formyltetrahydrofolate deformylase                             |
| R714 | One carbon pool by folate            | 1.5.1.3   | ABAYE3315 OR<br>ABAYE3614 OR<br>ABAYE3644 | THF + NAD <-> DHF + NADH   | dihydrofolate reductase  |
| R715 | One carbon pool by folate            | 1.5.1.3   | ABAYE3315 OR<br>ABAYE3614 OR<br>ABAYE3644 | THF + NADP <-> DHF + NADPH   | dihydrofolate reductase  |
| R716 | Porphyrin and chlorophyll metabolism | 1.2.1.70  | ABAYE2976                                 | GTRNA + NADPH -> GSA + NADP  | glutamyl-tRNA reductase  |
| R717 | Porphyrin and chlorophyll metabolism | 5.4.3.8   | ABAYE1011                                 | GSA -> ALAV  | glutamate-1-semialdehyde aminotransferase                      |
| R718 | Porphyrin and chlorophyll metabolism | 4.2.1.24  | ABAYE2909                                 | 2 ALAV -> PBG  | porphobilinogen synthase                                       |
| R719 | Porphyrin and chlorophyll metabolism | 2.5.1.61  | ABAYE3508                                 | 4 PBG -> HMB + 4 NH3   | hydroxymethylbilane synthase                                   |
| R720 | Porphyrin and chlorophyll metabolism | 4.2.1.75  | ABAYE3507                                 | HMB -> UPRG  | uroporphyrinogen-III synthase                                  |
| R721 | Porphyrin and chlorophyll metabolism | 2.1.1.107 | ABAYE0758                                 | 2 SAM + UPRG -> 2 SAH + PC2  | uroporphyrin-III C-methyltransferase                           |
| R722 | Porphyrin and chlorophyll metabolism | 1.3.1.76  | ABAYE0758                                 | PC2 + NAD -> NADH + SHCL   | precorrin-2 dehydrogenase                                      |
| R723 | Porphyrin and chlorophyll metabolism | 4.99.1.4  | ABAYE0758                                 | SHCL -> SHEME  | sirohdrochlorin ferrochelatase                                 |
| R724 | Porphyrin and chlorophyll metabolism | 4.1.1.37  | ABAYE1106                                 | UPRG -> 4 CO2 + CPP  | uroporphyrinogen decarboxylase                                 |
| R725 | Porphyrin and chlorophyll metabolism | 1.3.99.22 | ABAYE0674 OR<br>ABAYE3379                 | CPP + 2 SAM -> PPHG + 2 CO2 + 2 MET + 2 DA   | oxygen-independent coproporphyrinogen III oxidase              |
| R726 | Porphyrin and chlorophyll metabolism | 1.3.3.3   | ABAYE0378                                 | CPP + O2 -> PPHG + 2 CO2   | coproporphyrinogen III oxidase                                 |
| R727 | Porphyrin and chlorophyll metabolism | 4.99.1.1  | ABAYE3393                                 | PPIX -> PTH  | ferrochelatase   |
| R728 | Porphyrin and chlorophyll metabolism | 2.5.1.17  | ABAYE0605                                 | C(I)DA + ATP -> ACDA + PPI + PI  | cob(I)alamin adenosyltransferase                               |
| R729 | Porphyrin and chlorophyll metabolism | 2.7.1.156 | ABAYE1994                                 | ADCBA + ATP -> ADCBAP + ADP  | adenosylcobinamide kinase                                      |
| R730 | Porphyrin and chlorophyll metabolism | 2.7.1.156 | ABAYE1994                                 | ADCBA + GTP -> ADCBAP + GDP  | adenosylcobinamide kinase                                      |
| R731 | Porphyrin and chlorophyll metabolism | 2.7.1.156 | ABAYE1994                                 | ADCBAP + GTP -> AGDPCBA + PPI  | adenosylcobinamide-phosphate guanylyltransferase               |
| R732 | Porphyrin and chlorophyll metabolism | 2.7.8.26  | ABAYE1990                                 | AGDPCBA + ARBZ -> CBCO + GMP   | adenosylcobinamide-GDP ribazoletransferase                     |
| R733 | Porphyrin and chlorophyll metabolism | 2.5.1.17  | ABAYE0605                                 | ATP + CBA <-> PPPI + ADCBA   | cob(I)alamin adenosyltransferase                               |
| R734 | Porphyrin and chlorophyll metabolism | 2.5.1.17  | ABAYE0605                                 | ATP + C(I)A <-> PPPI + CBCO  | cob(I)alamin adenosyltransferase                               |
| R735 | Porphyrin and chlorophyll metabolism | 4.1.1.37  | ABAYE1106                                 | UPRGI <-> CPPI + 4 CO2   | uroporphyrinogen decarboxylase                                 |
| R736 | Porphyrin and chlorophyll metabolism | 2.5.1.-   | ABAYE1385                                 | PTH <-> HEMEO  | protoheme IX farnesyltransferase                               |
| R737 | Ubiquinone biosynthesis              | 5.4.4.2   | ABAYE1104                                 | CHOR <-> ICHOR   | menaquinone-specific isochorismate synthase                    |
| R738 | Ubiquinone biosynthesis              | 4.1.3.40  | ABAYE1127                                 | CHOR <-> 4HB + PYR   | chorismate--pyruvate lyase                                     |
| R739 | Ubiquinone biosynthesis              | 2.5.1.-   | ABAYE1128                                 | OPP + 4HB -> 3OP4HB + PPI  | 4-hydroxybenzoate octaprenyltransferase                        |
| R740 | Ubiquinone biosynthesis              | UbIB      | ABAYE3426                                 | 2OPP + O2 + NADPH -> 2OP6HP + NADP   | ubiquinone biosynthesis protein                                |
| R741 | Ubiquinone biosynthesis              | 2.1.1.64  | ABAYE3834                                 | 2OP6HP + SAM -> 2OP6MP + SAH   | 3-demethylubiquinone-9 3-methyltransferase                     |
| R742 | Ubiquinone biosynthesis              | 1.14.13.- | ABAYE2678                                 | 2OP6MP + O2 + NADPH -> 2OP6M14BQ + NADP  | 2-octaprenyl-6-methoxyphynol hydroxylase                       |
| R743 | Ubiquinone biosynthesis              | 2.1.1.-   | ABAYE3424                                 | 2OP6M14BQ + SAM -> 2OP3M6M14BQ + SAH   | 2-octaprenyl-6-methoxy-1,4-benzoquinone methylase              |
| R744 | Ubiquinone biosynthesis              | 2.1.1.64  | ABAYE3834                                 | 2OP3M5H6M14BQ + SAM -> UQ + SAH  | 3-demethylubiquinone-9 3-methyltransferase                     |
| R745 | Ubiquinone biosynthesis              | 2.5.1.64  |   | ICHOR + AKG -> SHCHC + PYR + CO2   | 2-succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate synthase |
| R746 | Ubiquinone biosynthesis              | 4.2.1.-   |   | SHCHC -> OSB   | O-succinylbenzoate-CoA synthase                                |
| R747 | Ubiquinone biosynthesis              | 6.2.1.26  |   | OSB + ATP + COA -> AMP + PPI + OSBCOA  | O-succinylbenzoic acid--CoA ligase                             |
| R748 | Ubiquinone biosynthesis              | 4.1.3.36  |   | OSBCOA -> DHN + COA  | dihydroxynaphthoic acid synthase                               |
| R749 | Ubiquinone biosynthesis              | 2.5.1.-   | ABAYE1128                                 | DHN + OPP -> PPI + CO2 + DMK   | 4-hydroxybenzoate octaprenyltransferase                        |
| R750 | Ubiquinone biosynthesis              | 2.1.1.-   | ABAYE3424                                 | DMK + SAM -> MKH2 + SAH  | menaquinone biosynthesis methyltransferase                     |
| R751 | Ubiquinone biosynthesis              | 2.1.1.-   | ABAYE3424                                 | 2P14NQ + SAM -> PQ + SAH   | menaquinone biosynthesis methyltransferase                     |
| R752 | Ubiquinone biosynthesis              | 1.14.13.- | ABAYE1427                                 | 2HP3M6M14B + O2 + NADPH <-> 2HP3M5H6M14B + NADP  | ubiquinone biosynthesis protein                                |
| R753 | Protein                              |           |   | 0.488 ALA + 0.281 ARG + 0.229 ASN + 0.229 ASP + 0.087 CYS + 0.25 GLU + 0.25 GLN + 0.582 GLY + 0.09 HIS + 0.276 ILE + 0.428 LEU + 0.326 LYS + 0.146 MET + 0.176 PHE + 0.21 PRO + 0.205 SER + 0.241 THR + 0.054 TRP + 0.131 TYR + 0.402 VAL + 40 ATP -> 40 ADP + 40 PI + PROTEIN |  |
| R754 | DNA                                  | 2.7.7.7   |   | 0.987 DATP + 0.631 DGTP + 0.631 DCTP + 0.987 DTTT + 4.4 ATP -> 4.4 ADP + 4.4 PI + 3.237 PPI + DNA  |  |
| R755 | RNA                                  | 2.7.7.6   |   | 2.045 ATP + 0.920 GTP + 0.686 CTP + 0.689 UTP -> 1.25 ADP + 1.25 PI + 3.091 PPI + RNA  |  |
| R756 | Phospholipid                         |           |   | 0.168 CL + 0.548 PE + 0.302 PG + 0.12 2AG3PE -> PHOSPHOLIPID   |  |
| R757 | Lipids                               |           |   | 0.058 C100ACP + 0.185 C120ACP + 0.013 C140ACP + 0.012 C150ACP + 1.082 C160ACP + 0.74 C161ACP + 0.067 C170ACP + 0.06 C171ACP + 0.032 C180ACP + 1.443 C181ACP + 0.157 C120OH -> LIPID + 3.692 ACP  |  |
| R758 | Lipopolysaccharide biosynthesis      |           |   | 0.182 KDO + 0.821 bDGLC + 0.656 UDPGAL + 0.018 DTDPRMNS + 0.365 UDPNAG + 0.255 UDPAGLACA + 0.037 C120ACP + 0.014 C160ACP + 0.079 C120OH + 0.009 C180ACP + 0.008 C181ACP + 0.071 C140OH -> LPS + 1.276 UDP + 0.018 DTD + 0.068 ACP  |  |
| R759 |                                      |           |   | 2.794 DTDPRMNS + 2.117 bDGLC + 0.265 GDPMAN -> EXOPOLYS + 2.794 DTD + 0.265 UDP  |  |
| R760 | Cofactors and vitamins (CAV)         |           |   | 0.163 COA + 0.159 FAD + 0.274 FMN + 0.405 MK + 0.188 NAD + 0.168 NADP + 0.739 PYRDX + 0.281 THF -> CAV   |  |
| R761 | Biomass                              |           |   | 0.6 PROTEIN + 0.03 DNA + 0.19 RNA + 0.04 PHOSPHOLIPID + 0.02 LIPID + 0.005 LPS + 0.027 PEPTIDO + 0.038 EXOPOLYS + 0.03 CAV + 46 ATP -> BIOMASS + 46 ADP + 46 PI  |  |

| No.  | Metabolism          | EC Number | ORF | Reaction                         | Enzyme |
|------|---------------------|-----------|-----|----------------------------------|--------|
| R762 | Maintenance         |           |     | ATP -> ADP + PI                  |        |
| R763 | IMAL_transport      | 3.6.1.-   |     | IMALxt + ATP <-> IMAL + PI + ADP |        |
| R764 | FRU_transport       | 2.7.1.69  |     | FRUxt + PEP -> F1P + PYR         |        |
| R765 | GLC_transport       |           |     | GLCxt + ATP -> GLC + ADP + PI    |        |
| R766 | GLUC_transport      |           |     | GLUCxt + Hxt -> GLUC             |        |
| R767 | MLT_transport       |           |     | MLTxt + ATP -> MLT + ADP + PI    |        |
| R768 | MNT_transport       |           |     | MNTxt + ATP -> MNT + ADP + PI    |        |
| R769 | NAGA_transport      |           |     | NAGxt + ATP -> NAGA + ADP + PI   |        |
| R770 | SUC_transport       |           |     | SUCxt + ATP -> SUC + ADP + PI    |        |
| R771 | TRE_transport       |           |     | TRExt + ATP -> TRE + ADP + PI    |        |
| R772 | 2PG_transport       |           |     | 2PGxt + ATP -> 2PG + ADP + PI    |        |
| R773 | 3PG_transport       |           |     | 3PGxt + ATP -> 3PG + ADP + PI    |        |
| R774 | AC_transport        |           |     | AC <-> ACxt + Hxt                |        |
| R775 | AKG_transport       |           |     | AKGxt + Hxt -> AKG               |        |
| R776 | AKG_transport       |           |     | AKGxt + Naxt -> AKG + Na         |        |
| R777 | CIT_transport       |           |     | CITxt <-> CIT                    |        |
| R778 | FORMATE_transport   |           |     | FORMATE -> FORMATExt             |        |
| R779 | FUM_transport       |           |     | FUMxt + Hxt -> FUM               |        |
| R780 | FUM_transport       |           |     | FUMxt + Naxt -> FUM + Na         |        |
| R781 | FUM_transport       |           |     | FUMxt + SUCC <-> FUM + SUCCxt    |        |
| R782 | ICIT_transport      |           |     | ICITxt + Naxt -> ICIT + Na       |        |
| R783 | MAL_transport       |           |     | MALxt + Hxt -> MAL               |        |
| R784 | MAL_transport       |           |     | MALxt + Naxt -> MAL + Na         |        |
| R785 | MAL_transport       |           |     | MALxt + SUCC <-> MAL + SUCCxt    |        |
| R786 | SLAC_transport      |           |     | SLACxt + Hxt -> SLAC             |        |
| R787 | SUCC_transport      |           |     | SUCCxt + Hxt -> SUCC             |        |
| R788 | SUCC_transport      |           |     | SUCCxt + Naxt -> SUCC + Na       |        |
| R789 | GLYCOLATE_transport |           |     | GLYCOLATExt <-> GLYCOLATE        |        |
| R790 | ATP_transport       |           |     | ATP <-> Hxt + ADP + PI           |        |
| R791 | CO2_transport       |           |     | CO2xt <-> CO2                    |        |
| R792 | Na_transport        |           |     | Naxt <-> Na + Hxt                |        |
| R793 | NH3_transport       |           |     | NH3xt <-> NH3                    |        |
| R794 | NO2_transport       |           |     | NO2 -> NO2xt                     |        |
| R795 | NO3_transport       |           |     | NO3xt + ATP -> NO3 + ADP + PI    |        |
| R796 | O2_transport        |           |     | O2xt <-> O2                      |        |
| R797 | PI_transport        |           |     | PIxt + Hxt <-> PI                |        |
| R798 | PI_transport        |           |     | PIxt + ATP -> 2 PI + ADP         |        |
| R799 | SLF_transport       |           |     | SLFxt + Hxt -> SLF               |        |
| R800 | SLF_transport       |           |     | SLFxt + ATP -> SLF + ADP + PI    |        |
| R801 | ALA_transport       |           |     | ALA + Hxt <-> ALAxt              |        |
| R802 | ALA_transport       |           |     | ALAxt + ATP -> ALA + ADP + PI    |        |
| R803 | ALA_transport       |           |     | ALAxt + Hxt -> ALA               |        |
| R804 | ALA_transport       |           |     | ALAxt + Naxt -> ALA + Na         |        |
| R805 | ARG_transport       |           |     | ARG + Hxt <-> ARGxt              |        |
| R806 | ARG_transport       |           |     | ARGxt + ATP -> ARG + ADP + PI    |        |
| R807 | ARG_transport       |           |     | ARGxt + Hxt -> ARG               |        |
| R808 | ASN_transport       |           |     | ASN + Hxt <-> ASNxt              |        |
| R809 | ASN_transport       |           |     | ASNxt + ATP -> ASN + ADP + PI    |        |
| R810 | ASN_transport       |           |     | ASNxt + Hxt -> ASN               |        |
| R811 | ASP_transport       |           |     | ASP + Hxt <-> ASPxt              |        |
| R812 | ASP_transport       |           |     | ASPxt + ATP -> ASP + ADP + PI    |        |
| R813 | ASP_transport       |           |     | ASPxt + Hxt -> ASP               |        |
| R814 | CYS_transport       |           |     | CYS + Hxt <-> CYSxt              |        |
| R815 | CYS_transport       |           |     | CYSxt + ATP -> CYS + ADP + PI    |        |
| R816 | CYS_transport       |           |     | CYSxt + Hxt -> CYS               |        |
| R817 | DALA_transport      |           |     | DALAXt + Hxt -> DALA             |        |
| R818 | DGLU_transport      |           |     | DGLUxt + Hxt -> DGLU             |        |
| R819 | GLN_transport       |           |     | GLN + Hxt <-> GLNxt              |        |
| R820 | GLN_transport       |           |     | GLNxt + ATP -> GLN + ADP + PI    |        |
| R821 | GLN_transport       |           |     | GLNxt + Hxt -> GLN               |        |
| R822 | GLU_transport       |           |     | GLU + Hxt <-> GLUxt              |        |
| R823 | GLU_transport       |           |     | GLUxt + ATP -> GLU + ADP + PI    |        |
| R824 | GLU_transport       |           |     | GLUxt + Hxt -> GLU               |        |
| R825 | GLU_transport       |           |     | GLUxt + Naxt -> GLU + Na         |        |
| R826 | GLY_transport       |           |     | GLY + Hxt <-> GLYxt              |        |
| R827 | GLY_transport       |           |     | GLYxt + ATP -> GLY + ADP + PI    |        |
| R828 | GLY_transport       |           |     | GLYxt + Hxt -> GLY               |        |
| R829 | GLY_transport       |           |     | GLYxt + Naxt -> GLY + Na         |        |
| R830 | HIS_transport       |           |     | HIS + Hxt <-> HISxt              |        |
| R831 | HIS_transport       |           |     | HISxt + ATP -> HIS + ADP + PI    |        |
| R832 | HIS_transport       |           |     | HISxt + Hxt -> HIS               |        |
| R833 | ILE_transport       |           |     | ILE + Hxt <-> ILExt              |        |
| R834 | ILE_transport       |           |     | ILExt + ATP -> ILE + ADP + PI    |        |
| R835 | ILE_transport       |           |     | ILExt + Hxt -> ILE               |        |
| R836 | LEU_transport       |           |     | LEU + Hxt <-> LEUxt              |        |
| R837 | LEU_transport       |           |     | LEUxt + ATP -> LEU + ADP + PI    |        |
| R838 | LEU_transport       |           |     | LEUxt + Hxt -> LEU               |        |
| R839 | LYS_transport       |           |     | LYS + Hxt <-> LYSxt              |        |
| R840 | LYS_transport       |           |     | LYS + Hxt -> LYSxt               |        |
| R841 | LYS_transport       |           |     | LYSxt + ATP -> LYS + ADP + PI    |        |
| R842 | LYS_transport       |           |     | LYSxt + Hxt -> LYS               |        |
| R843 | MET_transport       |           |     | MET + Hxt <-> METxt              |        |
| R844 | MET_transport       |           |     | METxt + ATP -> MET + ADP + PI    |        |
| R845 | MET_transport       |           |     | METxt + Hxt -> MET               |        |
| R846 | PHE_transport       |           |     | PHE + Hxt <-> PHExt              |        |
| R847 | PHE_transport       |           |     | PHExt + ATP -> PHE + ADP + PI    |        |
| R848 | PHE_transport       |           |     | PHExt + Hxt -> PHE               |        |
| R849 | PRO_transport       |           |     | PRO + Hxt <-> PROxt              |        |
| R850 | PRO_transport       |           |     | PROxt + ATP -> PRO + ADP + PI    |        |
| R851 | PRO_transport       |           |     | PROxt + Hxt -> PRO               |        |
| R852 | PRO_transport       |           |     | PROxt + Naxt -> PRO + Na         |        |
| R853 | SER_transport       |           |     | SER + Hxt <-> SERxt              |        |
| R854 | SER_transport       |           |     | SERxt + ATP -> SER + ADP + PI    |        |
| R855 | SER_transport       |           |     | SERxt + Hxt -> SER               |        |
| R856 | THR_transport       |           |     | THR + Hxt <-> THRxt              |        |
| R857 | THR_transport       |           |     | THRxt + ATP -> THR + ADP + PI    |        |
| R858 | THR_transport       |           |     | THRxt + Hxt -> THR               |        |
| R859 | TRP_transport       |           |     | TRP + Hxt <-> TRPxt              |        |
| R860 | TRP_transport       |           |     | TRPxt + ATP -> TRP + ADP + PI    |        |
| R861 | TRP_transport       |           |     | TRPxt + Hxt -> TRP               |        |
| R862 | TYR_transport       |           |     | TYR + Hxt <-> TYRxt              |        |
| R863 | TYR_transport       |           |     | TYRxt + ATP -> TYR + ADP + PI    |        |
| R864 | TYR_transport       |           |     | TYRxt + Hxt -> TYR               |        |
| R865 | VAL_transport       |           |     | VAL + Hxt <-> VALxt              |        |

| No.  | Metabolism        | EC Number | ORF | Reaction                          | Enzyme |
|------|-------------------|-----------|-----|-----------------------------------|--------|
| R866 | VAL_transport     |           |     | VALxt + ATP -> VAL + ADP + PI     |        |
| R867 | VAL_transport     |           |     | VALxt + Hxt -> VAL                |        |
| R868 | DSER_transport    |           |     | DSERxt + Hxt -> DSER              |        |
| R869 | ARG_transport     |           |     | ARGxt + ORN <-> ARG + ORNxt       |        |
| R870 | HSER_transport    |           |     | HSER + Hxt <-> HSERxt             |        |
| R871 | ORN_transport     |           |     | ORNxt + ATP -> ORN + ADP + PI     |        |
| R872 | PTRC_transport    |           |     | PTRCxt + ATP -> PTRC + ADP + PI   |        |
| R873 | SPRMD_transport   |           |     | SPRMDxt + ATP -> SPRMD + ADP + PI |        |
| R874 | UREA_transport    |           |     | UREAxt + ATP -> UREA + ADP + PI   |        |
| R875 | CHOLINE_transport |           |     | CHOLINExt + Hxt -> CHOLINE        |        |
| R876 | ADN_transport     |           |     | ADNxt + Hxt -> ADN                |        |
| R877 | CYTD_transport    |           |     | CYTDxt + Hxt -> CYTD              |        |
| R878 | DA_transport      |           |     | DAxt + Hxt -> DA                  |        |
| R879 | DC_transport      |           |     | DCxt + Hxt -> DC                  |        |
| R880 | DG_transport      |           |     | DGxt + Hxt -> DG                  |        |
| R881 | DT_transport      |           |     | DTxt + Hxt -> DT                  |        |
| R882 | DU_transport      |           |     | DUxt + Hxt -> DU                  |        |
| R883 | GSN_transport     |           |     | GSNxt + Hxt -> GSN                |        |
| R884 | URI_transport     |           |     | URIXt + Hxt -> URI                |        |
| R885 | CT_transport      |           |     | CTxt + Hxt -> CT                  |        |
| R886 | XAN_transport     |           |     | XANxt + Hxt -> XAN                |        |
| R887 | URA_transport     |           |     | URAXt + Hxt -> URA                |        |
| R888 | TR_transport      |           |     | TRxt + ATP -> TR + ADP + PI       |        |
| R889 | ETHA_transport    |           |     | ETHAXt + Hxt -> ETHA              |        |
| R890 | BETAINE_transport |           |     | BETAINExt + Hxt -> BETAINE        |        |
| R891 | BZ_transport      |           |     | BZxt + Hxt -> BZ                  |        |

Supplementary Table 2. Metabolites participating in reactions of AbyMBEL891.

| Metabolite abbreviations | Metabolite names   |
|--------------------------|--|
| (2AE)P                   | (2-Aminoethyl)phosphonate  |
| 13DAP                    | 1,3-Diaminopropane; Trimethylenediamine; 1,3-Propanediamine; Propane-1,3-diamine   |
| 13PDG                    | 3-Phospho-D-glyceroyl phosphate  |
| 1BOH                     | 1-Butanol  |
| 2(HE)TPP                 | 2-(alpha-Hydroxyethyl)thiamine diphosphate   |
| 23BOH                    | (R,R)-Butane-2,3-diol; (R,R)-2,3-Butanediol; (R,R)-2,3-Butylene glycol   |
| 24DAB                    | L-2,4-Diaminobutanoate   |
| 2AA                      | 2-Aminoacrylate  |
| 2AG3PC                   | 2-Acyl-sn-glycero-3-phosphocholine   |
| 2AG3PE                   | 2-Acyl-sn-glycero-3-phosphoethanolamine; L-1-Lysophosphatidylethanolamine  |
| 2AG3PS                   | 2-Acyl-sn-glycero-3-phosphoserine  |
| 2AGL3P                   | 2-Acyl-sn-glycerol 3-phosphate   |
| 2H3OSUCC                 | 2-Hydroxy-3-oxosuccinate; Oxaloglycolate   |
| 2HP3M5H6M14B             | 2-Hexaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinone   |
| 2HP3M6M14B               | 2-Hexaprenyl-3-methyl-6-methoxy-1,4-benzoquinone   |
| 2HPA                     | 2-Hydroxyphenylacetate   |
| 2HPP                     | 2-Hydroxypropylphosphonate   |
| 2MAACCOA                 | 2-Methylacetoacetyl-CoA  |
| 2MB2ECCOA                | 2-Methylbut-2-enoyl-CoA  |
| 2MBCOA                   | (S)-2-Methylbutanoyl-CoA   |
| 2MCIT                    | 2-Methylcitrate  |
| 2MP2ECCOA                | 2-Methylprop-2-enoyl-CoA   |
| 2MPPACOA                 | 2-Methylpropanoyl-CoA  |
| 2NPRPN                   | 2-Nitropropane   |
| 2OAD                     | 2-Oxoadipate   |
| 2OP3M5H6M14BQ            | 2-Octaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinone   |
| 2OP3M6M14BQ              | 2-Octaprenyl-3-methyl-6-methoxy-1,4-benzoquinone   |
| 2OP6HP                   | 2-Octaprenyl-6-hydroxyphenol   |
| 2OP6M14BQ                | 2-Octaprenyl-6-methoxy-1,4-benzoquinone  |
| 2OP6MP                   | 2-Octaprenyl-6-methoxyphenol   |
| 2OPP                     | 2-Octaprenylphenol   |
| 2P14NQ                   | 2-Phytyl-1,4-naphthoquinone  |
| 2P1A                     | 2-Propyn-1-ol  |
| 2PCDPMDE                 | 2-Phospho-4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol  |
| 2PG                      | 2-Phospho-D-glycerate  |
| 2PPG                     | 2-Phosphoglycolate   |
| 34DHB                    | 3,4-Dihydroxybenzoate; 3,4-Dihydroxybenzoic acid; Protocatechuate; Protocatechuic acid   |
| 34DHMA                   | 3,4-Dihydroxymandelaldehyde  |
| 34DHPA                   | 3,4-Dihydroxyphenylacetate   |
| 34DHPEG                  | 3,4-Dihydroxyphenylethyleneglycol  |
| 3A2OP                    | 3-Amino-2-oxopropyl phosphate  |
| 3AP                      | 3-Aminopropanal; beta-Aminopropion aldehyde  |
| 3B1A                     | 3-Butyn-1-ol   |
| 3BUT                     | 3-Butynoate  |
| 3DDAH7P                  | 2-Dehydro-3-deoxy-D-arabino-heptonate 7-phosphate  |
| 3H2MBCOA                 | (2S,3S)-3-Hydroxy-2-methylbutanoyl-CoA   |
| 3H3MGCCOA                | (S)-3-Hydroxy-3-methylglutaryl-CoA   |
| 3HAN                     | 3-Hydroxyanthranilate  |
| 3HB123TC                 | (2S,3R)-3-Hydroxybutane-1,2,3-tricarboxylate   |
| 3HBCOA                   | (S)-3-Hydroxybutanoyl-CoA  |
| 3HBUT                    | (R)-3-Hydroxybutanoate; (R)-3-Hydroxybutyric acid  |
| 3HIBCOA                  | (S)-3-Hydroxyisobutyryl-CoA  |
| 3HIVCOA                  | 3-Hydroxyisovaleryl-CoA  |
| 3HPA                     | 3-Hydroxyphenylacetate   |
| 3HPCOA                   | 3-Hydroxypropionyl-CoA   |
| 3MBCOA                   | 3-Methylbutanoyl-CoA   |
| 3MCCOA                   | 3-Methylcrotonyl-CoA   |
| 3MGCCOA                  | 3-Methylglutaconyl-CoA   |
| 3MOP                     | (S)-3-Methyl-2-oxopentanoic acid; (S)-3-Methyl-2-oxopentanoate; (3S)-3-Methyl-2-oxopentanoic acid; (3S)-3-Methyl-2-oxopentanoate |
| 3OP4HB                   | 3-Octaprenyl-4-hydroxybenzoate   |
| 3OPP                     | 3-Oxopropanoate; Malonate semialdehyde   |
| 3PG                      | 3-Phospho-D-glycerate  |
| 3PSER                    | 3-Phosphoserine  |
| 3PSME                    | 5-O-(1-Carboxyvinyl)-3-phosphoshikimate  |
| 3SFPYR                   | 3-Sulfinylpyruvate   |
| 3SLALA                   | 3-Sulfino-L-alanine  |
| 3SPYR                    | 3-Sulfoxyruvate  |
| 4AABUT                   | 4-Acetamidobutanoate   |
| 4AB                      | 4-Aminobutanal   |
| 4FAAC                    | 4-Fumarylacetoacetate  |
| 4GBTA                    | 4-Guanidinobutanamide  |
| 4GBTR                    | 4-Guanidinobutanoate; 4-Guanidinobutyric acid  |
| 4HB                      | 4-Hydroxybenzoate  |
| 4HGLUSA                  | L-4-Hydroxyglutamate semialdehyde  |
| 4HLT                     | 4-Hydroxy-L-threonine  |
| 4HMN                     | 4-Hydroxymandelonitrile  |
| 4HPA                     | 4-Hydroxyphenylacetate   |
| 4HPACAL                  | 4-Hydroxyphenylacetaldehyde; 2-(4-Hydroxyphenyl)acetaldehyde   |
| 4HPACALO                 | (Z)-4-Hydroxyphenylacetaldehyde-oxime  |
| 4HPACOA                  | 4-Hydroxyphenylacetyl-CoA  |
| 4HPAGLY                  | 4-Hydroxyphenylacetyl-glycine  |
| 4HPP                     | 3-(4-Hydroxyphenyl)pyruvate  |
| 4HPRO                    | trans-4-Hydroxy-L-proline  |
| 4I5P                     | 4-Imidazole-5-propanoate   |
| 4MAAC                    | 4-Maleylacetoacetate   |
| 4MOP                     | 4-Methyl-2-oxopentanoate   |
| 4PPNCYS                  | (R)-4'-Phosphopantothenoyl-L-cysteine  |
| 4PPNTE                   | Pantetheine 4'-phosphate   |
| 4PPNTO                   | D-4'-Phosphopantothenate   |
| 4TMABT                   | 4-Trimethylammoniobutanal  |
| 4TMABTO                  | 4-Trimethylammoniobutanoate  |
| 5A4ICA                   | 5-Amino-4-imidazole carboxylate  |
| 5AI                      | 5-Aminoimidazole; Aminoimidazole; 4-Aminoimidazole   |
| 5C2O3E                   | 5-Carboxy-2-oxohept-3-enedioate  |
| 5CM2HM                   | 5-Carboxymethyl-2-hydroxyruconate  |
| 5GLUPEPT                 | (5-L-Glutamyl)-peptide   |
| 5HIAA                    | 5-Hydroxyindoleacetaldehyde  |
| 5HIAC                    | 5-Hydroxyindoleacetate   |
| 5MC                      | DNA 5-methylcytosine; DNA containing 5-methylcytosine; 5-Methylcytosine (in DNA)   |
| 5MDR                     | 5-Methylthio-D-ribose  |

| Metabolite abbreviations | Metabolite names  |
|--------------------------|---|
| SMTA                     | 5-Methylthioadenosine   |
| SMTGLU                   | 5-Methyltetrahydropteroyltri-L-glutamate  |
| A[C]                     | Apo-[carboxylase]   |
| A5P                      | D-Arabinose 5-phosphate   |
| A6RP                     | 5-Amino-6-ribitylamino-2,4 (1H, 3H)-pyrimidinedione; 4-(1-D-Ribitylamino)-5-amino-2,6-dihydropyrimidine; 4-(1-D-Ribitylamino)-5-aminouracil   |
| A6RP5P                   | 5-Amino-6-(5'-phosphoribosylamino)uracil  |
| A6RP5P2                  | 5-Amino-6-(5'-phosphoribitylamino)uracil  |
| AAA                      | Aminoacetaldehyde   |
| AAC                      | Acetoacetate  |
| AACCOA                   | Acetoacetyl-CoA   |
| AACTN                    | Aminoacetone; 1-Amino-2-propanone   |
| AAD                      | Acetyl adenylate  |
| ABUT                     | (S)-2-Aceto-2-hydroxybutanoate  |
| AC                       | Acetate   |
| ACACP                    | Acetyl-[acyl-carrier protein]   |
| ACAL                     | Acetaldehyde  |
| ACCOA                    | Acetyl-CoA  |
| ACDA                     | Adenosyl cobyriinate a,c diamide  |
| ACETYLP                  | Acetyl phosphate  |
| ACLAC                    | 2-Acetolactate  |
| ACOA                     | Acyl-CoA  |
| ACP                      | Acyl-carrier protein  |
| ACT                      | (R)-Acetoin; (R)-2-Acetoin; (R)-3-Hydroxy-2-butanone; (R)-Dimethylketol; (R)-3-Hydroxybutan-2-one   |
| ACTN                     | Acetone; Dimethyl ketone; 2-Propanone   |
| AD                       | Adenine   |
| ADCBA                    | Adenosyl cobinamide   |
| ADCBAP                   | Adenosyl cobinamide phosphate   |
| ADCHOR                   | 4-amino-4-deoxychorismate   |
| ADLIPO                   | 6-S-Acetyldihydroliipoamide; [Dihydroliipoalysine-residue acetyltransferase] S-acetyldihydroliipoalysine; S-Acetyldihydroliipoamide-E   |
| ADN                      | Adenosine   |
| ADP                      | ADP   |
| AEIOH                    | 3-(2-Aminoethyl)-1H-indol-5-ol; Serotonin; 5-Hydroxytryptamine; Enteramine  |
| AG                       | L-Arogenate   |
| AGDPCBA                  | Adenosine-GDP-cobinamide  |
| AGL                      | Acylglycerol  |
| AGL3P                    | 1-Acyl-sn-glycerol 3-phosphate  |
| AHMD                     | 2-Amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)pteridine   |
| AHHMP                    | 2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine  |
| AHM                      | 4-Amino-5-hydroxymethyl-2-methylpyrimidine  |
| AHMP                     | 4-Amino-5-hydroxymethyl-2-methylpyrimidine-phosphate  |
| AHMPP                    | 4-Amino-5-hydroxymethyl-2-methylpyrimidine-pyrophosphate  |
| AHTD                     | 2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)dihydropteridine triphosphate; 6-(L-erythro-1,2-Dihydroxypropyl 3-triphosphate)-7,8-dihydropterin; 6-[(1S,2R)-1,2-Dihydroxy-3-triphosphoxypropyl]-7,8-dihydropterin; 7,8-Dihydroneopterin 3'-triphosphate |
| AIBUT                    | L-3-Amino-isobutanoate; (S)-3-Amino-isobutyrate; L-3-Amino-isobutyrate; (S)-3-Amino-isobutanoate; (S)-3-Amino-2-methylpropanoate  |
| AICAR                    | 1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxamide  |
| AIR                      | Aminoimidazole ribotide   |
| AKG                      | 2-Oxoglutarate  |
| ALA                      | L-Alanine   |
| ALAALA                   | D-alanyl-D-alanine  |
| ALATRNA                  | L-Alanyl-tRNA   |
| ALAV                     | D-Aminolevulinate   |
| ALLNT                    | Allantoate; Allantoic acid  |
| AMP                      | AMP   |
| AN                       | Anthranilate  |
| AONA                     | 8-amino-7-oxononanoate  |
| APN                      | beta-Aminopropionitrile; 3-Aminopropionitrile   |
| AppppA                   | P1,P4-Bis(5'-adenosyl) tetraphosphate   |
| APS                      | Adenylylsulfate; Adenylyl sulfate; Adenosine 5'-phosphosulfate; APS; 5'-Adenylyl sulfate  |
| ARBZ                     | alpha-Ribazole; N1-(alpha-D-ribose)-5,6-dimethylbenzimidazole   |
| ARG                      | L-Arginine  |
| ARGSUCC                  | N-(L-Arginino)succinate   |
| ARGTRNAARG               | L-Arginyl-tRNA(Arg)   |
| ARIB                     | ADPribose   |
| ASELNT                   | Adenylylselenate  |
| ASER                     | O-Acetyl-L-serine   |
| ASN                      | L-Asparagine  |
| ASNTRNAASN               | L-Asparaginyl-tRNA(Asn)   |
| ASP                      | L-Aspartate   |
| ASPSA                    | L-Aspartate 4-semialdehyde  |
| ASPTRNAASN               | L-Aspartyl-tRNA(Asn)  |
| ASPTRNAASP               | L-Aspartyl-tRNA(Asp)  |
| ASUC                     | N6-(1,2-Dicarboxyethyl)-AMP   |
| ATP                      | ATP   |
| B5AMP                    | Biotinyl-5'-AMP   |
| BAL                      | Betaine aldehyde  |
| bALA                     | beta-Alanine  |
| bAPA                     | beta-Aminopropion aldehyde  |
| BASP                     | 4-Phospho-L-aspartate   |
| bDG6P                    | beta-D-Glucose 6-phosphate  |
| bDGLC                    | beta-D-Glucose  |
| BETAINE                  | Betaine; Glycine betaine  |
| BT                       | Biotin  |
| BUTANAL                  | Butanal   |
| BZ                       | Benzoate; Benzoic acid; Benzenecarboxylic acid; Phenylformic acid; Dracylic acid  |
| C(I)A                    | Cob(I)alamin; Cbl; Vitamin B12s   |
| C(I)DA                   | Cob(I)yrinate a,c diamide   |
| C090ACP                  | Nonanoyl-[acyl-carrier protein]   |
| C100                     | Decanoic acid   |
| C100ACP                  | Decanoyl-[acyl-carrier protein]   |
| C110ACP                  | Undecanoyl-[acyl-carrier protein]   |
| C120                     | Dodecanoic acid   |
| C120ACP                  | Dodecanoyl-[acyl-carrier protein]   |
| C120OH                   | beta-hydroxy dodecanoic acid  |
| C121COA                  | cis,cis-3,6-Dodecadienoyl-CoA   |
| C122COA                  | trans,cis-Lauro-2,6-dienoyl-CoA   |
| C130ACP                  | Tridecanoyl-[acyl-carrier protein]  |
| C140                     | Tetradecanoic acid  |
| C140ACP                  | Tetradecanoyl-[acyl-carrier protein]  |



| Metabolite abbreviations | Metabolite names  |
|--------------------------|---|
| C14OOH                   | beta-hydroxy tetradecanoic acid   |
| C150                     | Pentadecanoic acid  |
| C150ACP                  | Pentadecanoyl-[acyl-carrier protein]  |
| C151ACP                  | Pentadecenoyl-[acyl-carrier protein]  |
| C160                     | Hexadecanoic acid   |
| C160ACP                  | Hexadecanoyl-[acyl-carrier protein]   |
| C161                     | Hexadecenoic acid   |
| C161ACP                  | Hexadecenoyl-[acyl-carrier protein]   |
| C170                     | Heptadecanoic acid  |
| C170ACP                  | Heptadecanoyl-[acyl-carrier protein]  |
| C171                     | Heptadecenoic acid  |
| C171ACP                  | Heptadecenoyl-[acyl-carrier protein]  |
| C180                     | Octadecanoic acid   |
| C180ACP                  | Octadecanoyl-[acyl-carrier protein]   |
| C181                     | Octadecenoic acid   |
| C181ACP                  | Octadecenoyl-[acyl-carrier protein]   |
| C190ACP                  | Nonadecanoyl-[acyl-carrier protein]   |
| C191ACP                  | Nonadecenoyl-[acyl-carrier protein]   |
| C200ACP                  | Eicosanoyl-[acyl-carrier protein]   |
| CAASP                    | N-Carbamoyl-L-aspartate   |
| CAIR                     | 1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate                                      |
| CALA                     | 3-Cyano-L-alanine; L-3-Cyanoalanine; L-beta-Cyanoalanine                                    |
| CAP                      | Carbamoyl phosphate   |
| CATECHOL                 | Catechol; 1,2-Benzenediol; o-Benzenediol; 1,2-Dihydroxybenzene; Brenzcatechin; Pyrocatechol |
| CAV                      | Cofactors and vitamins  |
| CBA                      | Cobinamide  |
| CBCO                     | Cobamide coenzyme   |
| CBHCAP                   | 3-Isopropylmalate   |
| CCOA                     | Crotonoyl-CoA   |
| CDHDI                    | 2-Carboxy-2,3-dihydro-5,6-dihydroxyindole   |
| CDP                      | CDP   |
| CDPDG                    | CDP-diacylglycerol  |
| CDPMDE                   | 4-(Cytidine 5'-diphospho)-2-C-methyl-D-erythritol   |
| CH3OR                    | Primary alcohol   |
| CHCOA                    | 6-carboxyhexanoyl-CoA; Pimeloyl-CoA   |
| CHITB                    | Chitobiose  |
| CHOLINE                  | Choline   |
| CHOLINEP                 | Choline phosphate; Phosphorylcholine; Phosphocholine; O-Phosphocholine                      |
| CHOR                     | Chorismate  |
| CIT                      | Citrate   |
| CITR                     | L-Citrulline  |
| CL                       | Cardiolipin (biomass component)   |
| CMP                      | CMP   |
| CMPAEP                   | CMP-2-aminoethylphosphonate; CMPciliate   |
| CMPKDO                   | CMP-2-keto-3-deoxyoctanoate   |
| CNS                      | Carnosine   |
| CO2                      | CO2   |
| COA                      | CoA; coenzyme A   |
| CPAD5P                   | 1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose 5-phosphate                                     |
| CPP                      | Coproporphyrinogen III  |
| CPPI                     | Coproporphyrinogen I  |
| CRTN                     | Creatine; alpha-Methylguanidino acetic acid; Methylglycocyanine                             |
| CT                       | DNA cytosine; Cytosine (in DNA)   |
| CTP                      | CTP   |
| CVN                      | Cinnavalinate   |
| CYS                      | L-Cysteine  |
| CYSGLY                   | Cys-Gly; L-Cysteinyglycine  |
| CYST                     | L-Cystine   |
| CYSTEATE                 | L-Cysteate  |
| CYSTRNACYS               | L-Cysteinyl-tRNA(Cys)   |
| CYTD                     | Cytidine  |
| D6PGC                    | 6-Phospho-D-gluconate   |
| D6RP5P                   | 2,5-Diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine                                 |
| D8RL                     | 6,7-Dimethyl-8-(1-D-ribityl)lumazine  |
| DA                       | Deoxyadenosine  |
| DAC                      | Diacetyl; Biacetyl; Dimethylglyoxal; 2,3-Butanedione  |
| DADP                     | dADP  |
| DALA                     | D-alanine   |
| DAMP                     | dAMP  |
| DANNA                    | 7,8-Diaminononanoate  |
| DAPIM                    | LL-2,6-Diaminopimelate  |
| DASP                     | D-Aspartate   |
| DATP                     | dATP  |
| DB4P                     | L-3,4-Dihydroxy-2-butanone 4-phosphate  |
| DC                       | Deoxycytidine   |
| DCDP                     | dCDP  |
| DCMP                     | dCMP  |
| DCTP                     | dCTP  |
| DCYS                     | D-Cysteine; D-Amino-3-mercaptopropionic acid  |
| DG                       | Deoxyguanosine  |
| DGDP                     | dGDP  |
| DGLN                     | D-Glutamine   |
| DGLU                     | D-Glutamate   |
| DGLUCA                   | D-Glucarate   |
| DGLUCL                   | D-Glucuronolactone  |
| DGLYCERATE               | D-glycerate   |
| DGMP                     | dGMP  |
| DGR                      | 1,2-Diacyl-sn-glycerol; 1,2-Diacylglycerol  |
| DGTP                     | dGTP  |
| DHAP                     | Glycerone phosphate   |
| DHDP                     | 2,3-Dihydrodipicolinate   |
| DHF                      | Dihydrofolate   |
| DHI                      | 5,6-Dihydroxyindole   |
| DHLIPOYLPROTEIN          | Dihydrolipeoylprotein   |
| DHMP                     | (R)-2,3-dihydroxy-3-methylpentanoate  |
| DHMVA                    | (R)-2,3-dihydroxy-3-methylbutanoate   |
| DHN                      | 1,4-dihydroxy-2-naphthoate  |
| DHP                      | 2-Amino-4-hydroxy-6-(D-erythro-1,2,3-trihydroxypropyl)-7,8-dihydropteridine                 |
| DHPA                     | 2,6-Dihydroxyphenylacetate  |
| DHPACAL                  | 3,4-Dihydroxyphenylacetaldehyde; Protocatechuatealdehyde                                    |
| DHPANT                   | 2-Dehydropantoate   |
| DHPT                     | Dihydropteroate   |
| DHSK                     | 3-Dehydroshikimate  |

| Metabolite abbreviations | Metabolite names   |
|--------------------------|--|
| DIDP                     | dIDP   |
| DIMGP                    | D-erythro-1-(imidazol-4-yl)glycerol 3-phosphate  |
| DIMP                     | 2'-Deoxyinosine 5'-phosphate; dIMP   |
| DIN                      | Deoxyinosine   |
| DISAC1P                  | 2,3-bis(3-hydroxytetradecanoyl)-D-glucosaminyl-1,6-beta-D-2,3-bis(3-hydroxytetradecanoyl)-beta-D-glucosaminyl 1-phosphate or disaccharide 1-P  |
| DITP                     | dITP   |
| DLIPO                    | Enzyme N6-(dihydrolipoyl)lysine; Dihydrolipoamide-E  |
| DMB                      | Dimethylbenzimidazole  |
| DMK                      | 2-Demethylmenaquinone  |
| DMKH2                    | 2-Demethylmenaquinol   |
| DMPP                     | Dimethylallyl diphosphate  |
| DNA                      | DNA (biomass component)  |
| DOROA                    | (S)-Dihydroorotate   |
| DPCHR                    | L-Dopachrome; 2-L-Carboxy-2,3-dihydroindole-5,6-quinone  |
| DPCOA                    | Dephospho-CoA  |
| DPHE                     | D-Phenylalanine  |
| DPM                      | Dopamine; 4-(2-Aminoethyl)-1,2-benzenediol; 4-(2-Aminoethyl)benzene-1,2-diol; 3,4-Dihydroxyphenethylamine; 2-(3,4-Dihydroxyphenyl)ethylamine   |
| DPRO                     | D-Proline  |
| DQT                      | 3-Dehydroquinate   |
| DR1P                     | 2-Deoxy-D-ribose 1-phosphate   |
| DR5P                     | 2-Deoxy-D-ribose 5-phosphate   |
| DSER                     | D-Serine   |
| DT                       | Thymidine  |
| DTB                      | Deithiobiotin  |
| DTDP                     | dTDP   |
| DTDP4O6DG                | 4,6-Dideoxy-4-oxo-dTDP-D-glucose; dTDP-4-oxo-6-deoxy-D-glucose; dTDP-4-dehydro-6-deoxy-D-glucose; dTDP-4-dehydro-6-deoxy-alpha-D-glucose; dTDP-4-oxo-6-deoxy-alpha-D-glucose; dTDP-4-dehydro-6-deoxy-alpha-D-galactose; dTDP-4-dehydro-6-deoxy-D-galactose |
| DTDP4ORMNS               | dTDP-4-dehydro-6-deoxy-L-mannose; dTDP-4-oxo-6-deoxy-L-mannose; dTDP-4-oxo-L-rhamnose  |
| DTDPGLAC                 | dTDPgalactose  |
| DTDPGLU                  | dTDP-glucose; dTDP-D-glucose; dTDP-alpha-D-glucose   |
| DTDPRMNS                 | dTDP-6-deoxy-L-mannose; dTDP-L-rhamnose  |
| DTMP                     | dTMP   |
| DTTP                     | dTTP   |
| DU                       | Deoxyuridine   |
| DUDP                     | dUDP   |
| DUMP                     | dUMP   |
| DUTP                     | dUTP   |
| DX5P                     | 1-Deoxy-D-xylulose 5-phosphate   |
| E4HGLU                   | L-erythro-4-Hydroxyglutamate   |
| E4P                      | D-Erythrose 4-phosphate  |
| ER4P                     | 4-Phospho-D-erythronate; 4-Phosphoerythronate  |
| ETH                      | Ethanol  |
| ETHA                     | Ethanolamine   |
| ETHAP                    | Ethanolamine phosphate; O-Phosphorylethanolamine; Phosphoethanolamine; O-Phosphoethanolamine   |
| EXOPOLYS                 | Exopolysaccharide  |
| F1P                      | D-Fructose 1-phosphate   |
| F6P                      | beta-D-Fructose 6-phosphate  |
| FA                       | Formamide  |
| FAD                      | Flavin adenine dinucleotide; FAD   |
| FADH2                    | FADH2  |
| FAN                      | Formylanthranilate; N-Formylanthranilate; 2-(Formylamino)-benzoic acid   |
| FDP                      | beta-D-Fructose 1,6-bisphosphate   |
| FERIC                    | Ferricytochrome c  |
| FEROC                    | Ferrocyclochrome c   |
| FGAM                     | 2-(Formamido)-N1-(5'-phosphoribosyl)acetamidine  |
| FGAR                     | 5'-Phosphoribosyl-N-formylglycinamide  |
| FKYN                     | L-Formylkynurenine; N-Formyl-L-kynurenine; N-Formylkynurenine  |
| FL                       | Folate   |
| FMETTRNA                 | N-Formylmethionyl-tRNA   |
| FMN                      | FMN; Riboflavin-5-phosphate; Flavin mononucleotide   |
| FORMATE                  | Formate  |
| FPP                      | trans,trans-Farnesyl diphosphate   |
| FTHF                     | 10-Formyltetrahydrofolate  |
| FUCP                     | L-Fucose 1-phosphate   |
| FUM                      | Fumarate   |
| G1P                      | D-Glucose 1-phosphate  |
| G3P                      | D-Glyceraldehyde 3-phosphate; (2R)-2-Hydroxy-3-(phosphonoxy)-propanal  |
| G3PC                     | sn-glycero-3-Phosphocholine  |
| G3PE                     | sn-glycero-3-Phosphoethanolamine   |
| G6P                      | alpha-D-Glucose 6-phosphate  |
| GA1P                     | D-Glucosamine 1-phosphate  |
| GA6P                     | D-Glucosamine 6-phosphate  |
| GABA                     | 4-Aminobutanoate   |
| GAPN                     | gamma-Glutamyl-beta-aminopropionitrile; gamma-Glutamyl-3-aminopropionitrile  |
| GAR                      | 5'-Phosphoribosylglycinamide   |
| GCYS                     | gamma-L-Glutamyl-L-cysteine  |
| GDP                      | GDP  |
| GDPMAN                   | GDP-mannose  |
| GENAL                    | Gentisate aldehyde   |
| GGLUMSCYS                | gamma-Glutamyl-Se-methylselenocysteine   |
| GGPP                     | Geranylgeranyl diphosphate   |
| GL                       | Glycerol   |
| GL3P                     | sn-Glycerol 3-phosphate  |
| GLAL                     | Glycolaldehyde   |
| GLC                      | alpha-D-Glucose  |
| GLCA                     | D-Glucosamine; Chitosamine; 2-Amino-2-deoxy-D-glucose  |
| GLCAMN                   | D-Glucosaminide  |
| GLN                      | L-Glutamine  |
| GLU                      | L-Glutamate  |
| GLUBCALA                 | gamma-Glutamyl-beta-cyanoalanine   |
| GLUC                     | D-Gluconate  |
| GLUGSAL                  | L-Glutamate 5-semialdehyde   |
| GLUP                     | alpha-D-Glutamyl phosphate   |
| GLUTCOA                  | Glutamyl-CoA   |
| GLUTR                    | 5-L-Glutamyl-taurine   |
| GLUTRNAGLN               | L-Glutamyl-tRNA(Gln)   |
| GLUTRNAGLU               | L-Glutamyl-tRNA(Glu)   |
| GLX                      | Glyoxylate   |

| Metabolite abbreviations | Metabolite names  |
|--------------------------|---|
| GLY                      | Glycine   |
| GLYCOLATE                | Glycolate   |
| GLYTRNAGLY               | Glycyl-tRNA(Gly)  |
| GMP                      | GMP   |
| GN                       | Guanine   |
| GPP                      | Geranyl diphosphate   |
| GSA                      | Glutamate-1-semialdehyde  |
| GSN                      | Guanosine   |
| GTP                      | GTP   |
| GTRNA                    | GlutaminyI-tRNA   |
| H[C]                     | Holo-[carboxylase]  |
| H2O2                     | H2O2  |
| H2S                      | Hydrogen sulfide  |
| H2SO3                    | Sulfite   |
| H5P                      | Hydantoin-5-propionate; Hydantoin-propionate  |
| HAC                      | Hydroxyacetone  |
| HCNS                     | Homocarnosine   |
| HCO3                     | HCO3  |
| HCYS                     | L-Homocysteine  |
| HDN                      | Hordeanine; 4-[2-(Dimethylamino)ethyl]phenol  |
| HEDC                     | 2-Hydroxyethylenedicarboxylate; enol-Oxaloacetate; enol-Oxaloacetic acid; 2-Hydroxybut-2-enedioic acid  |
| HEMEO                    | Heme O  |
| HEPPP                    | all-trans-Heptaprenyl diphosphate   |
| HIBUT                    | (S)-3-Hydroxyisobutyrate  |
| HIEA                     | 1H-Imidazole-4-ethanamine; Histamine; 2-(4-Imidazolyl)ethylamine  |
| HIPPRT                   | Hippurate; Hippuric acid; N-Benzoylglycine; Benzoylaminoacetic acid   |
| HIS                      | L-Histidine   |
| HISOL                    | L-Histidinol  |
| HISOLP                   | L-Histidinol phosphate  |
| HISTRNAHIS               | L-Histidyl-tRNA(His)  |
| HKYN                     | 3-Hydroxy-L-kynurenine  |
| HMB                      | Hydroxymethylbilane   |
| HMB4PP                   | 1-Hydroxy-2-methyl-2-butenyl 4-diphosphate  |
| HO3S2                    | Thiosulfate   |
| HOMOGEN                  | Homogentisate   |
| HOPP                     | 2-Hydroxy-3-oxopropanoate; Tartronate semialdehyde  |
| HPYR                     | Hydroxypyruvate; Hydroxypyruvic acid; 3-Hydroxypyruvate; 3-Hydroxypyruvic acid  |
| HSER                     | L-Homoserine  |
| Hxt                      | External proton   |
| HYDROXYAKG               | D-4-Hydroxy-2-oxoglutarate  |
| HYNX                     | Hypoxanthine  |
| I3AA                     | Indole-3-acetaldehyde   |
| I3AAM                    | Indole-3-acetamide  |
| I3AC                     | Indole-3-acetate  |
| I4AA                     | Imidazole-4-acetaldehyde  |
| I4AC                     | Imidazole-4-acetate   |
| IASP                     | Iminoaspartate  |
| ICHOR                    | Isochorismate   |
| ICIT                     | Isocitrate  |
| IDP                      | IDP   |
| IGLY                     | Iminoglycine; Iminoacetic acid  |
| IGP                      | Indoleglycerol phosphate  |
| ILE                      | L-Isoleucine  |
| ILETRNAILE               | L-Isoleucyl-tRNA(Ile)   |
| IMACP                    | 3-(Imidazol-4-yl)-2-oxopropyl phosphate   |
| IMAL                     | Isomaltose  |
| IMP                      | IMP   |
| INDOLE                   | Indole  |
| INS                      | Inosine   |
| IPP                      | Isopentenyl diphosphate   |
| IPPMAL                   | 2-Isopropylmalate; (2S)-2-Isopropylmalate; 3-Carboxy-3-hydroxy-4-methylpentanoate; 3-Carboxy-3-hydroxy-isocaproate; 3-Carboxy-3-hydroxyisocaproate; 2-Hydroxy-2-isopropylbutanedioate; 3-Hydroxy-4-methyl-3-carboxypentanoate |
| IPYR                     | Indolepyruvate; Indolepyruvic acid; (Indol-3-yl)pyruvate; Indole-3-pyruvate; 3-(Indol-3-yl)pyruvate   |
| ITP                      | ITP   |
| K2LIPA                   | KDO2-lipid (A); Di[3-deoxy-D-manno-octulosonyl]-lipid A   |
| K2LPIV                   | KDO2-lipid IV(A); Di[3-deoxy-D-manno-octulosonyl]-lipid IV(A);  |
| KDO                      | 2-Dehydro-3-deoxy-D-octonate  |
| KDOLIPV                  | KDO-lipid IV(A)   |
| KDOP                     | 2-Dehydro-3-deoxy-D-octonate 8-phosphate  |
| KDPG                     | 2-Dehydro-3-deoxy-6-phospho-D-gluconate   |
| KYN                      | L-Kynurenine; 3-Anthraniloyl-L-alanine  |
| L1P3H5C                  | L-1-Pyrroline-3-hydroxy-5-carboxylate   |
| LAC                      | (R)-Lactate, D-Lactate  |
| LACAL                    | (S)-Lactaldehyde; L-Lactaldehyde; L-2-Hydroxypropionaldehyde  |
| LEU                      | L-Leucine   |
| LEUTRNA                  | L-Leucyl-tRNA   |
| LIPID                    | Lipids other than phospholipid  |
| LIPV                     | Lipid IV(A)   |
| LIPO                     | Enzyme N6-(lipoyl)lysine; Lipoamide-E   |
| LIPOLPROTEIN             | Lipoylprotein   |
| LIPX                     | Lipid X   |
| LK2LPIV                  | Lauroyl-KDO2-lipid IV(A)  |
| LLCT                     | L-Cystathionine   |
| LPS                      | Lippolysaccharide   |
| LTG                      | (R)-S-Lactoylglutathione  |
| LYS                      | L-Lysine  |
| LYSTRNA                  | L-Lysyl-tRNA  |
| MAL                      | (S)-Malate  |
| IMALCP                   | Malonyl-[acyl-carrier protein]  |
| MALCOA                   | Malonyl-CoA   |
| MAN1P                    | alpha-D-Mannose 1-phosphate   |
| MAN6P                    | D-Mannose 6-phosphate   |
| MCB                      | Methylcobalamin   |
| MDAPIM                   | meso-2,6-Diaminoheptanedioate; meso-2,6-Diaminopimelate; meso-2,6-Diaminopimelic acid; meso-Diaminoheptanedioate  |
| MDE4P                    | 2-C-Methyl-D-erythritol 4-phosphate   |
| MDECPP                   | 2-C-Methyl-D-erythritol 2,4-cyclodiphosphate  |
| MET                      | L-Methionine  |
| METHF                    | 5,10-Methylenetetrahydrofolate  |
| METTHF                   | 5,10-Methylenetetrahydrofolate  |
| METTRNA                  | L-Methionyl-tRNA  |

| Metabolite abbreviations | Metabolite names   |
|--------------------------|--|
| MK                       | menaquinone  |
| MKH2                     | menaquinol   |
| MLT                      | Maltose  |
| MM                       | Methylmalonate   |
| MMALCOA                  | (S)-Methylmalonyl-CoA; (S)-Methylmalonyl-coenzyme A; (2S)-Methylmalonyl-CoA; D-Methylmalonyl-CoA |
| MMSA                     | (S)-Methylmalonate semialdehyde  |
| MNT                      | D-Mannitol   |
| MOT                      | 5-Methoxytryptamine; 5-MeOT  |
| MPET                     | 4-Methyl-5-(2-phosphoethyl)-thiazole; 4-Methyl-5-(2-phosphono-oxethyl)-thiazole                  |
| MPYR                     | Mercaptopyruvate   |
| MSCYS                    | Se-Methylselenocysteine  |
| MTG                      | Methylglyoxal  |
| MTHF                     | 5-Methyltetrahydrofolate   |
| MTRM                     | N-Methyltyramine   |
| MTTA                     | meso-Tartaric acid; meso-Tartrate  |
| N(P)CYS                  | N-((R)-Pantothenoyl)-L-cysteine  |
| N1(5PADR)DMB             | N1-(5-Phospho-alpha-D-ribose)-5,6-dimethylbenzimidazole  |
| N2SUCCARG                | N2-Succinyl-L-arginine   |
| N2SUCCGLU                | N-Succinyl-L-glutamate; (2S)-2-(3-Carboxypropanoylamino)pentanedioic acid                        |
| N2SUCCGLU5SA             | N-Succinyl-L-glutamate 5-semialdehyde; (2S)-2-(3-Carboxypropanoylamino)-5-oxopentanoic acid      |
| N4AAB                    | N4-Acetylaminobutanal  |
| Na                       | Sodium   |
| NAAD                     | Deamino-NAD+; Deamido-NAD+; Deamido-NAD  |
| NAC                      | Nicotinate   |
| NACD                     | Nicotinate D-ribonucleoside  |
| NACN                     | Nicotinate D-ribonucleotide  |
| NAD                      | NAD+; Nicotinamide adenine dinucleotide  |
| NADH                     | NADH   |
| NADMA                    | N-Acetyl-D-mannosamine   |
| NADP                     | NADP+; Nicotinamide adenine dinucleotide phosphate   |
| NADPH                    | NADPH  |
| NAGA                     | N-Acetyl-D-glucosamine   |
| NAGA1P                   | N-Acetyl-D-glucosamine 1-phosphate   |
| NAGLU                    | N-Acetyl-L-glutamate   |
| NAGLUP                   | N-Acetyl-L-glutamate 5-phosphate   |
| NAGLUS                   | N-Acetyl-L-glutamate 5-semialdehyde  |
| NAM                      | Nicotinamide   |
| NAMD                     | N-RibosylNicotinamide  |
| NAMN                     | Nicotinamide D-ribonucleotide  |
| NAORN                    | N2-Acetyl-L-ornithine  |
| NAS                      | N-Acylsphingosine; Ceramide  |
| NASAEF                   | Ceramide 2-aminoethylphosphonate; Ceramide ciliate   |
| NFGLU                    | N-Formimino-L-glutamate  |
| NH3                      | NH3  |
| NHLYS                    | N6-Hydroxy-L-lysine  |
| NMHIS                    | N(pi)-Methyl-L-Histidine   |
| NO2                      | Nitrite  |
| NO3                      | Nitrate  |
| NPRAN                    | N-(5-Phospho-D-ribose)anthranilate   |
| O2                       | Oxygen   |
| OA                       | Oxaloacetate   |
| OAHSER                   | O-Acetyl-L-homoserine  |
| OBUT                     | 2-Oxobutanoate   |
| OCT                      | Oxidized glutathione; Glutathione disulfide; Oxiglutatione                                       |
| OHB                      | 3-Hydroxy-4-phospho-hydroxy-alpha-ketobutyrate   |
| OICAP                    | 3-Carboxy-4-methyl-2-oxopentanoate   |
| OIVAL                    | 3-Methyl-2-oxobutanoic acid  |
| OMP                      | Orotidine 5'-phosphate   |
| OPP                      | all-trans-Octaprenyl diphosphate   |
| ORBRDX                   | Oxidized rubredoxin  |
| ORN                      | L-Ornithine  |
| OROA                     | Orotate  |
| OSB                      | O-succinylbenzoate   |
| OSBCOA                   | O-succinylbenzoate-CoA   |
| OSLHSER                  | O-Succinyl-L-homoserine  |
| OTHIO                    | Thioredoxin disulfide; Oxidized thioredoxin; Thioredoxin sulfide                                 |
| P5C                      | (S)-1-Pyrroline-5-carboxylate  |
| P5P                      | Pyridoxine 5-phosphate; Pyridoxine phosphate   |
| PA                       | Phosphatidate; 1,2-Diacyl-sn-glycerol 3-phosphate  |
| PAA                      | 2-Phenylacetamide  |
| PABA                     | 4-Aminobenzoate  |
| PACAL                    | Phenylacetaldehyde; alpha-Tolualdehyde   |
| PACGLY                   | Phenylacetylglycine  |
| PACOA                    | Phenylacetyl-CoA   |
| PANT                     | (R)-pantoate   |
| PAP                      | Adenosine 3',5'-bisphosphate   |
| PAPS                     | 3'-Phosphoadenylyl sulfate   |
| PBG                      | Prophobilinogen  |
| PC                       | Phosphatidylcholine  |
| PC2                      | Percorrin 2  |
| PDLA                     | Pyridoxamine   |
| PDLA5P                   | Pyridoxamine-5-phosphate   |
| PE                       | Phosphatidylethanolamine   |
| PEA                      | Phenethylamine; 2-Phenylethylamine; beta-Phenylethylamine; Phenylethylamine                      |
| PEP                      | Phosphoenolpyruvate  |
| PEPTIDE                  | Peptide  |
| PEPTIDO                  | Peptidoglycan (biomass component)  |
| PG                       | Phosphatidylglycerol   |
| PGP                      | Phosphatidylglycerophosphate   |
| PHE                      | L-Phenylalanine  |
| PHEN                     | Prephenate   |
| PHETRNPHE                | L-Phenylalanyl-tRNA(Phe)   |
| PHOSPHOLIPID             | Phospholipids (biomass component)  |
| PHP                      | 3-Phosphonoxypruvate   |
| PHPYR                    | Phenylpyruvate   |
| PHSER                    | O-Phospho-L-homoserine   |
| PHT                      | O-Phospho-4-hydroxy-L-threonine  |
| PI                       | Orthophosphate   |
| PL                       | Pyridoxal  |
| PL5P                     | Pyridoxal 5-phosphate  |
| PLA                      | Phenylacetic acid; Benzylformic acid; Phenylacetate; Benzeneacetic acid                          |
| PNTD                     | (R)-Pantothenate; Pantothenate   |

| Metabolite abbreviations | Metabolite names   |
|--------------------------|--|
| PPA                      | Propinol adenylate   |
| PAAACP                   | Propanoyl-[acyl-carrier protein]; Propionyl-[acyl-carrier protein]   |
| PPAC                     | Phosphonoacetaldehyde  |
| PPACOA                   | Propanoyl-CoA; Propionyl-CoA   |
| PPCOA                    | Propenoyl-CoA; Acryloyl-CoA  |
| PPEPTIDO                 | Peptidoglycan precursor  |
| ppGpp                    | Guanosine 3',5'-bis(diphosphate)   |
| PPHG                     | Protoporphyrinogen IX  |
| PPI                      | Pyrophosphate, Diphosphate   |
| PPIX                     | Protoporphyrin IX  |
| PPN                      | Propynoate   |
| pppGpp                   | Guanosine 3'-diphosphate 5'-triphosphate   |
| PPPI                     | Triphosphate   |
| PPPP                     | all-trans-Pentaprenyl diphosphate  |
| PQ                       | Phylloquinone  |
| PQQ                      | Pyrrolo-quinoline quinone; Pyrroloquinoline-quinone; Pyrroloquinoline quinone; 4,5-Dioxo-4,5-dihydro-1H-pyrrolo[2,3-f]quinoline-2,7,9-tricarboxylate |
| PQQH2                    | Reduced pyrroloquinoline-quinone   |
| PRAM                     | 5-Phosphoribosylamine  |
| PRBAMP                   | N1-(5-Phospho-D-ribose)-AMP  |
| PRBATP                   | N1-(5-Phospho-D-ribose)-ATP  |
| PRFICA                   | 1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide   |
| PRFP                     | 5-(5-Phospho-D-ribosylaminoformimino)-1-(5-phosphoribosyl)-imidazole-4-carboxamide   |
| PRLP                     | N-(5'-Phospho-D-1'-ribuloylformimino)-5-amino-1-(5'-phospho-D-ribose)-4-imidazolecarboxamide   |
| PRO                      | L-Proline  |
| PROPANOATE               | Propanoate   |
| PROPIONYLP               | Propanoyl phosphate  |
| PROTEIN                  | Proteins   |
| PROTRNAPRO               | L-Prolyl-tRNA(Pro)   |
| PRPP                     | 5-Phospho-alpha-D-ribose 1-diphosphate   |
| PS                       | Phosphatidylserine   |
| PTH                      | Heme; Haem; Protoheme; Heme B; Protoheme IX  |
| PTRC                     | Putrescine   |
| PTT                      | Pantetheine  |
| PURI5P                   | Pseudouridine 5'-phosphate   |
| PYR                      | Pyruvate   |
| PYRDx                    | Pyridoxine   |
| PYTHP                    | 6-Pyruvoyltetrahydropterin   |
| QA                       | Quinolate; Pyridine-2,3-dicarboxylate  |
| QNT                      | Quinate; Quinic acid; Kinic acid; Chinic acid; L-Quinic acid; L-Quinate; (-)-Quinic acid   |
| R1P                      | D-Ribose 1-phosphate; alpha-D-Ribose 1-phosphate; Ribose 1-phosphate   |
| R3HBCOA                  | (R)-3-Hydroxybutanoyl-CoA  |
| R5P                      | D-Ribose 5-phosphate   |
| RCHO                     | Aldehyde   |
| RGT                      | Glutathione  |
| RH                       | Alkane   |
| RIBFLAV                  | Riboflavin   |
| RL5P                     | D-Ribulose 5-phosphate   |
| RMAL                     | (R)-Malate; D-Malate; D-Malic acid   |
| RNA                      | RNA  |
| RRBRDX                   | Reduced rubredoxin   |
| RTHIO                    | Thioredoxin  |
| S                        | Sulfur   |
| S6P                      | Sorbitol 6-phosphate   |
| S7P                      | Sedoheptulose 7-phosphate  |
| SAH                      | S-Adenosyl-L-homocysteine  |
| SAICAR                   | 1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole   |
| SAM                      | S-Adenosyl-L-methionine  |
| SAMOB                    | S-adenosyl-4-methylthio-2-oxobutanoate   |
| SAOPIM                   | N-Succinyl-2-amino-6-oxopimelate   |
| SASHCYS                  | Se-Adenosylselenohomocysteine  |
| SB1P                     | Sorbose 1-phosphate  |
| SCSN                     | Sarcosine; N-Methylglycine   |
| SCYS                     | Selenocysteine   |
| SDAPIM                   | N-Succinyl-L-2,6-diaminopimelate   |
| SDLIPO                   | S-Succinyl-dihydroliipoamide   |
| SeASMET                  | Se-Adenosylselenomethionine  |
| SELD                     | Selenide   |
| SELNT                    | Selenate   |
| SELT                     | Selenite   |
| SER                      | L-Serine   |
| SERTRNASER               | L-Seryl-tRNA(Ser)  |
| SGDHL                    | S-Glutaryldihydroliipoamide  |
| SHCHC                    | 2-succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate  |
| SHCL                     | Sirohydrochlorin   |
| SHCYS                    | Selenohomocysteine   |
| SHEME                    | Siroheme   |
| SLAC                     | (S)-Lactate  |
| SLF                      | Sulfate  |
| SLLCT                    | Selenocystathionine  |
| SME                      | Shikimate  |
| SME3P                    | Shikimate 3-phosphate  |
| SMET                     | Selenomethionine   |
| SMETTRNAMET              | Selenomethionyl-tRNA(Met)  |
| SORN                     | N2-Succinyl-L-ornithine; (2S)-5-Amino-2-(3-carboxypropanoylamino)pentanoic acid  |
| SPRMD                    | Spermidine   |
| SRLH                     | S-Ribosyl-L-homocysteine   |
| SSLCYS                   | S-Sulfo-L-cysteine   |
| SUC                      | Sucrose  |
| SUCC                     | Succinate  |
| SUCCOA                   | Succinyl-CoA   |
| SUCCSA                   | Succinate semialdehyde   |
| T3                       | D-Glyceraldehyde   |
| TCYS                     | Thiocysteine   |
| TDHDP                    | 2,3,4,5-Tetrahydrodipicolinate   |
| TGL                      | Triacylglycerol  |
| TGLU                     | Tetrahydropteroyltri-L-glutamate   |
| THF                      | Tetrahydrofolate   |
| THFG                     | Tetrahydrofolyl-[Glu(n)]   |
| THIAMIN                  | Thiamin  |
| THMP                     | Thiamin monophosphate  |

| Metabolite abbreviations | Metabolite names   |
|--------------------------|--|
| THMP                     | Thiamin diphosphate  |
| THR                      | L-Threonine  |
| THRTRNATHR               | L-Threonyl-tRNA(Thr)   |
| THZ                      | 5-(2-Hydroxyethyl)-4-methylthiazole; 4-Methyl-5-(2'-hydroxyethyl)-thiazole; 4-Methyl-5-(2-hydroxyethyl)-thiazole                                       |
| THZP                     | 4-Methyl-5-(beta-hydroxyethyl)thiazole phosphate   |
| TM                       | Thymine  |
| TR                       | Taurine  |
| TRE                      | alpha, alpha-Trehalose   |
| TRE6P                    | alpha, alpha'-Trehalose 6-phosphate  |
| TRM                      | Tyramine; 2-(p-Hydroxyphenyl)ethylamine  |
| TRNAALA                  | tRNA(Ala)  |
| TRNAARG                  | tRNA(Arg)  |
| TRNAASP                  | tRNA(Asp)  |
| TRNACYS                  | tRNA(Cys)  |
| TRNAGLN                  | tRNA(Gln)  |
| TRNAGLU                  | tRNA(Glu)  |
| TRNAGLY                  | tRNA(Gly)  |
| TRNAHIS                  | tRNA(His)  |
| TRNAILE                  | tRNA(Ile)  |
| TRNALEU                  | tRNA(Leu)  |
| TRNALYS                  | tRNA(Lys)  |
| TRNAMET                  | tRNA(Met)  |
| TRNAPHE                  | tRNA(Phe)  |
| TRNAPRO                  | tRNA(Pro)  |
| TRNASER                  | tRNA(Ser)  |
| TRNATHR                  | tRNA(Thr)  |
| TRNATRP                  | tRNA(Trp)  |
| TRNATYR                  | tRNA(Tyr)  |
| TRNAVAL                  | tRNA(Val)  |
| TRP                      | L-Tryptophan   |
| TRPTRNATRP               | L-Tryptophanyl-tRNA(Trp)   |
| TRYTRNATYR               | L-Tyrosyl-tRNA(Tyr)  |
| TTA                      | (R,R)-Tartaric acid; (R,R)-Tartrate; L-Tartaric acid; Tartaric acid; Tartrate; 2,3-Dihydroxybutanedioic acid; (2R,3R)-Tartaric acid; (+)-Tartaric acid |
| TYR                      | L-Tyrosine   |
| U1C                      | Urea-1-carboxylate; Allophanate; Allophanic acid   |
| UC                       | Urocanate  |
| UDCP                     | Undecaprenyl phosphate   |
| UDCPP                    | Undecaprenyl diphosphate   |
| UDGLYCOLATE              | (-)-Ureidoglycolate; (S)-Ureidoglycolate   |
| UDP                      | UDP  |
| UDPAGLACA                | UDP-N-acetyl-D-galactosamine   |
| UDPG                     | UDP-glucose  |
| UDPG23A                  | UDP-2,3-bis(3-hydroxytetradecanoyl)glucosamine   |
| UDPG2A                   | UDP-3-O-(3-hydroxytetradecanoyl)glucosamine  |
| UDPG2AA                  | UDP-3-O-(3-hydroxytetradecanoyl)-N-acetylglucosamine   |
| UDPGAL                   | UDP-D-galactose  |
| UDPLUC                   | UDP-glucuronate  |
| UDPMNLADGMD              | UDP-N-acetylmuramoyl-L-alanyl-D-gamma-glutamyl-meso-2,6-diaminopimelate  |
| UDPMNLADGMDDADA          | UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-6-carboxy-L-lysyl-D-alanyl-D-alanine  |
| UDPNADMA                 | UDP-N-acetyl-D-mannosamine   |
| UDPNADMAU                | UDP-N-acetyl-D-mannosaminouronate  |
| UDPNAG                   | UDP-N-acetyl-D-glucosamine   |
| UDPNAGEP                 | UDP-N-acetyl-3-(1-carboxyvinyl)-D-glucosamine  |
| UDPNAM                   | UDP-N-acetylmuramate   |
| UDPNAMA                  | UDP-N-acetylmuramoyl-L-alanine   |
| UDPNAMAG                 | UDP-N-acetylmuramoyl-L-alanyl-D-glutamate  |
| UMP                      | UMP  |
| UPPMN(GN)LADGMDDADA      | Undecaprenyl-diphospho-N-acetylmuramoyl-(N-acetylglucosamine)-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine                          |
| UPPMN(GN)LADGNMD(G)5DA   | Undecaprenyl-diphospho-N-acetylmuramoyl-(N-acetylglucosamine)-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-(glycyl)5-D-alanyl-D-alanine                |
| UPPMN(GN)LADGNMDDADA     | Undecaprenyl-diphospho-N-acetylmuramoyl-(N-acetylglucosamine)-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine                          |
| UPPMNLADGMDDADA          | Undecaprenyl-diphospho-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine  |
| UPRG                     | Uroporphyrinogen III   |
| UPRGI                    | Uroporphyrinogen I   |
| UQ                       | Ubiquinone   |
| UQH2                     | Ubiquinol  |
| URA                      | Uracil   |
| UREA                     | Urea   |
| URI                      | Uridine  |
| URT                      | Urate; Uric acid   |
| UTP                      | UTP  |
| VAL                      | L-Valine   |
| VALTRNAVAL               | L-Valyl-tRNA(Val)  |
| VB12                     | Vitamin B12  |
| X5P                      | D-Xylulose 5-phosphate   |
| XAN                      | Xanthine   |
| XMP                      | Xanthosine 5'-phosphate  |
| XTP                      | XTP  |
| XTSINE                   | Xanthosine   |
| BIOMASS                  | Cell biomass   |
| FRUxt                    | External D-fructose  |

**Supplementary Table 3.** Biomass composition of *Acinetobacter baumannii*. Abbreviations are shown in parenthesis next to each macromolecule.

Supplementary Table 3A. Macromolecular composition. Macromolecular composition of *A. baumannii* AYE was adopted from various sources, including its close species, *A. calcoaceticus*, *A. baylyi*, and other *Acinetobacter* species as well as *Escherichia coli*.

| Component                    | Composition (g/g DCW) | References and comments   |
|------------------------------|-----------------------|---------------------------|
| Protein (PROTEIN)            | 0.600                 | 1                         |
| DNA (DNA)                    | 0.030                 | 2                         |
| RNA (RNA)                    | 0.190                 | 2                         |
| Phospholipids (PHOSPHOLIPID) | 0.040                 | 3                         |
| Fatty acids (LIPID)          | 0.020                 | 1                         |
| Lipopolysaccharide (LPS)     | 0.005                 | 4                         |
| Peptidoglycan (PEPTIDO)      | 0.027                 | 4                         |
| Exopolysaccharide (EXOPOLYS) | 0.038                 | 5                         |
| Cofactors and vitamins (CAV) | 0.030                 | -                         |
| Ash                          | 0.019                 | Not included in the model |
| Sum                          | 1.000                 |                           |

Supplementary Table 3B. Amino acid composition. Amino acid composition was adopted from that of *E. coli*<sup>6</sup>, based on the idea that amino acid composition does not affect enzyme and metabolite essentiality.

| Amino acids         | mmol/g protein |
|---------------------|----------------|
| Alanine (ALA)       | 0.488          |
| Arginine (ARG)      | 0.281          |
| Asparagine (ASN)    | 0.229          |
| Aspartate (ASP)     | 0.229          |
| Cystein (CYS)       | 0.087          |
| Glutamate (GLU)     | 0.250          |
| Glutamine (GLN)     | 0.250          |
| Glycine (GLY)       | 0.582          |
| Histidine (HIS)     | 0.090          |
| Isoleucine (ILE)    | 0.276          |
| Leucine (LEU)       | 0.428          |
| Lysine (LYS)        | 0.326          |
| Methionine (MET)    | 0.146          |
| Phenylalanine (PHE) | 0.176          |
| Proline (PRO)       | 0.210          |
| Serine (SER)        | 0.205          |
| Threonine (THR)     | 0.241          |
| Tryptophan (TRP)    | 0.054          |
| Tyrosine (TYR)      | 0.131          |
| Valine (VAL)        | 0.402          |

Supplementary Table 3C. DNA composition. DNA composition was determined from the genomic sequence of *A. baumannii* AYE at Genome database of NCBI (<http://www.ncbi.nlm.nih.gov/>). GC content of *A. baumannii* AYE is 39% <sup>7</sup>.

| Nucleotide | mol/mol, DNA | MW, g/mol | mmol/g DNA |
|------------|--------------|-----------|------------|
| dAMP       | 0.305        | 313.2065  | 0.987      |
| dGMP       | 0.195        | 329.2059  | 0.631      |
| dCMP       | 0.195        | 289.1818  | 0.631      |
| dTMP       | 0.305        | 304.1932  | 0.987      |

Supplementary Table 3D. RNA composition. It was assumed that mRNA makes up 5% and rRNA 80% of the total RNA. The rest was assumed to be tRNA <sup>8</sup>.

| Nucleotide | mol/mol RNA |          |          | MW, g/mol | mol/mol RNA | mmol/g RNA |
|------------|-------------|----------|----------|-----------|-------------|------------|
|            | 5% mRNA     | 80% rRNA | 15% tRNA |           |             |            |
| AMP        | 0.305       | 0.265    | 0.198    | 329.206   | 0.257       | 0.795      |
| GMP        | 0.195       | 0.303    | 0.305    | 345.205   | 0.298       | 0.920      |
| CMP        | 0.195       | 0.214    | 0.274    | 305.181   | 0.222       | 0.686      |
| UMP        | 0.305       | 0.218    | 0.223    | 306.166   | 0.223       | 0.689      |

Supplementary Table 3E. Phospholipid composition <sup>9</sup>.

| Component                                 | MW, g/mol, general structure | No. fatty acids | MW, g/mol, total phospholipids | mmol/g phospholipids |
|---|------------------------------|-----------------|--------------------------------|----------------------|
| Cardiolipin (CL) <sup>a</sup>             | 508.219                      | 4               | 1547.174                       | 0.168                |
| Phosphatidylethanolamine (PE)             | 269.146                      | 2               | 788.623                        | 0.548                |
| Phosphatidylglycerol (PG)                 | 300.157                      | 2               | 819.634                        | 0.302                |
| L-1-Lysophosphatidylethanolamine (2AG3PE) | 242.144                      | 1               | 501.882                        | 0.120                |

<sup>a</sup>Lysocardiolipin was also treated as cardiolipin as its molecular information was not available.

Supplementary Table 3F. Composition of fatty acids (LIPID) <sup>10</sup>.

| Fatty acid                         | g/g total fatty acids | MW, g/mol | mmol/g LIPID | mol/mol LIPID |
|------------------------------------|-----------------------|-----------|--------------|---------------|
| C10:0 (C100ACP)                    | 0.010                 | 172.265   | 0.058        | 0.015         |
| C12:0 (C120ACP)                    | 0.037                 | 200.318   | 0.185        | 0.048         |
| C14:0 (C140ACP)                    | 0.003                 | 228.371   | 0.013        | 0.003         |
| C15:0 (C150ACP)                    | 0.003                 | 242.398   | 0.012        | 0.003         |
| C16:0 (C160ACP)                    | 0.276                 | 256.424   | 1.082        | 0.281         |
| C16:1 (C161ACP) <sup>a</sup>       | 0.188                 | 254.408   | 0.740        | 0.192         |
| C17:0 (C170ACP)                    | 0.018                 | 270.451   | 0.067        | 0.017         |
| C17:1 (C171ACP)                    | 0.016                 | 268.435   | 0.060        | 0.016         |
| C18:0 (C180ACP)                    | 0.009                 | 284.477   | 0.032        | 0.008         |
| C18:1 (C181ACP) <sup>b</sup>       | 0.406                 | 282.461   | 1.443        | 0.375         |
| 2-OH C12:0OH (C120OH) <sup>c</sup> | 0.034                 | 217.327   | 0.157        | 0.041         |

<sup>a</sup>C16:1(9t), C16:1(7c) and C16:1(9c) in Yamahira et al. (2008) are combined together.

<sup>b</sup>C18:1(9t) and C18:1(9c) in Yamahira et al. (2008) are combined together.

<sup>c</sup>2-OH C12:0 and 3-OH C12:0 in Yamahira et al. (2008) are combined together.



Supplementary Table 3G. Lipopolysaccharide (LPS) composition <sup>4, 11</sup>. Metabolites included in AbyMBEL891 that closely resemble LPS components were selected for LPS formation: beta-D-glucose for glucose, UDP-N-acetyl-D-glucosamine for glucosamine, UDP-D-galactose for galactose and UDP-N-acetyl-D-galactosamine for galactosamine <sup>11</sup>.

| Component   | Molar ratio | MW, g/mol | mmol/g LPS |
|---|-------------|-----------|------------|
| 2-Dehydro-3-deoxy-D-octonate (KDO)                    | 1.0         | 238.192   | 0.182      |
| beta-D-Glucose (bDGLC) <sup>a</sup>                   | 4.5         | 180.156   | 0.821      |
| UDP-D-galactose (UDPGAL) <sup>a</sup>                 | 3.6         | 566.302   | 0.656      |
| dTDP-L-rhamnose (DTDPRMNS)                            | 0.1         | 548.330   | 0.018      |
| UDP-N-acetyl-D-glucosamine (UDPAG) <sup>b</sup>       | 2.0         | 607.354   | 0.365      |
| UDP-N-acetyl-D-galactosamine (UDPAGLACA) <sup>b</sup> | 1.4         | 607.354   | 0.255      |
| Dodecanoic acid (C120ACP) <sup>c</sup>                | 0.2         | 199.308   | 0.037      |
| Hexadecanoic acid (C160ACP) <sup>c</sup>              | 0.1         | 255.414   | 0.014      |
| beta-hydroxy dodecanoic acid (C120OH) <sup>c</sup>    | 0.4         | 216.317   | 0.079      |
| Octadecanoic acid (C180ACP) <sup>c</sup>              | 0.1         | 283.467   | 0.009      |
| Octadecenoic acid (C181ACP) <sup>c</sup>              | 0.0         | 281.451   | 0.008      |
| beta-hydroxy tetradecanoic acid (C140OH) <sup>c</sup> | 0.4         | 245.218   | 0.071      |

<sup>a</sup>These two molecules account for hexoses of LPS in Thorne et al. (1973).

<sup>b</sup>These two molecules account for hexosamines of LPS in Thorne et al. (1973).

<sup>c</sup>These fatty acids account for total fatty acids of LPS in Thorne et al. (1973).

Supplementary Table 3H. Exopolysaccharide (EXOPOLYS) composition <sup>5</sup>. Similar to LPS formation, metabolites included in AbyMBEL891 that closely resemble EXOPOLYS components were selected for its formation: dTDP-L-rhamnose for rhamnose, beta-D-Glucose for glucose and GDP-mannose for mannose.

| Component                  | Relative sugar composition (% w/w) | MW, g/mol | mmol/g EXOPOLYS |
|----------------------------|------------------------------------|-----------|-----------------|
| dTDP-L-rhamnose (DTDPRMNS) | 0.459                              | 164.157   | 2.794           |
| beta-D-Glucose (bDGLC)     | 0.381                              | 180.156   | 2.117           |
| GDP-mannose (GDPMAN)       | 0.160                              | 603.325   | 0.265           |

Supplementary Table 3I. Cofactors and vitamins (CAV) incorporated in the biomass. Cofactors and vitamins are assumed to be the same ratio (w/w).

| Molecule                          | MW, g/mol | g/g CAV | mmol/g CAV |
|-----------------------------------|-----------|---------|------------|
| Coenzyme A (COA)                  | 767.535   | 0.125   | 0.163      |
| Flavin adenine dinucleotide (FAD) | 785.550   | 0.125   | 0.159      |
| Flavin mononucleotide (FMN)       | 456.344   | 0.125   | 0.274      |
| Menaquinone (MK)                  | 308.414   | 0.125   | 0.405      |
| NAD                               | 664.433   | 0.125   | 0.188      |
| NADP                              | 744.413   | 0.125   | 0.168      |
| Pyridoxine (PYRDX)                | 169.178   | 0.125   | 0.739      |
| Tetrahydrofolate (THF)            | 445.430   | 0.125   | 0.281      |

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**Supplementary Table 4.** List of 246 essential reactions predicted under minimal medium with succinate as a sole carbon source. Information of each reaction is available in Supplementary Table 1.

| Reaction number of essential enzymes   |
|--|
| R001, R005, R006, R007, R008, R009, R010, R011, R012, R019, R020, R021, R025, R030, R031, R033, R035, R036, R044, R045, R046, R049, R050, R052, R053, R055, R056, R057, R058, R062, R063, R066, R068, R069, R070, R071, R095, R108, R143, R156, R157, R158, R159, R160, R162, R163, R164, R165, R167, R169, R171, R172, R174, R175, R176, R177, R178, R179, R183, R184, R185, R186, R187, R188, R189, R190, R191, R192, R203, R227, R231, R232, R234, R235, R237, R238, R239, R244, R245, R246, R248, R249, R250, R251, R252, R253, R254, R255, R256, R257, R258, R277, R278, R279, R281, R282, R299, R300, R303, R304, R305, R309, R310, R311, R312, R313, R314, R316, R320, R327, R328, R329, R331, R338, R346, R352, R356, R357, R361, R364, R375, R381, R382, R384, R413, R414, R415, R416, R417, R418, R421, R422, R423, R428, R431, R432, R433, R434, R435, R465, R466, R467, R468, R469, R470, R471, R472, R473, R501, R523, R524, R525, R526, R527, R528, R529, R532, R533, R534, R538, R539, R541, R548, R549, R550, R554, R555, R556, R557, R558, R559, R560, R571, R572, R591, R593, R608, R609, R610, R612, R613, R614, R615, R616, R617, R618, R619, R620, R621, R622, R632, R633, R634, R635, R636, R637, R638, R639, R640, R642, R643, R644, R646, R647, R648, R649, R651, R655, R656, R662, R665, R672, R673, R674, R675, R678, R679, R680, R681, R688, R690, R692, R693, R696, R708, R737, R745, R746, R747, R748, R749, R750, R753, R754, R755, R756, R757, R758, R759, R760, R761, R789, R791, R793, R796, R826 |

**Supplementary Table 5.** List of 681 reactions considered for comparison of their essentiality in AbyMBEL891 with those from *Acinetobacter baylyi* ADP1, which ultimately gave simulation-based prediction consistency of 72%. If essentiality of a reaction, either essential or non-essential, from AbyMBEL891 and ADP1 is the same, then they were considered consistent. This simulation was conducted under minimal medium with succinate as a sole carbon source. Information of each reaction is available in Supplementary Table 1.

| Reaction number of essential enzymes considered for comparative study   |
|---|
| R001, R002, R003, R004, R005, R006, R007, R008, R009, R010, R012, R013, R014, R015, R017, R018, R019, R020, R021, R022, R023, R024, R028, R030, R031, R034, R037, R038, R039, R040, R043, R044, R045, R047, R048, R049, R050, R053, R054, R056, R057, R058, R062, R063, R065, R066, R067, R068, R069, R070, R071, R072, R073, R074, R075, R076, R077, R078, R081, R082, R083, R084, R085, R088, R089, R090, R091, R092, R093, R094, R096, R097, R098, R101, R102, R103, R104, R106, R107, R110, R111, R112, R113, R115, R118, R119, R120, R121, R122, R123, R124, R125, R128, R129, R130, R131, R133, R135, R136, R137, R139, R140, R141, R142, R143, R144, R145, R146, R147, R148, R149, R150, R153, R154, R155, R156, R159, R160, R161, R162, R193, R194, R195, R196, R197, R198, R199, R200, R202, R203, R204, R208, R213, R215, R218, R219, R220, R221, R222, R223, R224, R225, R226, R228, R229, R230, R232, R233, R234, R235, R236, R237, R238, R240, R241, R242, R244, R245, R246, R247, R248, R249, R251, R252, R253, R254, R255, R256, R257, R258, R259, R260, R261, R262, R263, R264, R265, R266, R267, R268, R269, R273, R274, R275, R276, R277, R278, R279, R280, R281, R282, R284, R285, R286, R287, R289, R291, R298, R299, R303, R304, R305, R306, R307, R308, R309, R310, R312, R313, R314, R315, R316, R317, R318, R321, R322, R324, R325, R326, R327, R328, R329, R331, R332, R333, R338, R339, R340, R341, R342, R343, R344, R345, R347, R348, R349, R350, R351, R352, R353, R354, R355, R356, R357, R358, R359, R361, R362, R364, R365, R366, R367, R369, R371, R372, R373, R374, R375, R376, R377, R378, R380, R382, R384, R385, R386, R387, R388, R389, R390, R391, R392, R393, R394, R396, R397, R398, R399, R400, R401, R402, R404, R405, R407, R408, R409, R411, R412, R413, R414, R415, R418, R419, R420, R421, R422, R424, R425, R426, R427, R428, R429, R430, R431, R433, R434, R435, R436, R437, R438, R439, R440, R441, R444, R445, R446, R447, R448, R449, R450, R451, R452, R453, R454, R455, R456, R457, R458, R459, R460, R461, R462, R465, R467, R468, R469, R470, R471, R473, R475, R476, R481, R483, R484, R487, R488, R489, R490, R491, R492, R493, R494, R495, R497, R498, R499, R500, R501, R503, R504, R505, R507, R508, R509, R510, R512, R515, R516, R517, R518, R522, R523, R524, R525, R526, R527, R529, R530, R531, R533, R534, R535, R536, R537, R538, R539, R540, R542, R543, R544, R545, R546, R547, R549, R551, R552, R553, R554, R555, R556, R557, R558, R559, R560, R563, R564, R565, R566, R567, R569, R571, R572, R574, R577, R579, R581, R583, R584, R585, R586, R587, R588, R589, R590, R591, R592, R593, R594, R595, R596, R597, R598, R602, R603, R604, R605, R606, R607, R608, R609, R610, R611, R612, R613, R614, R615, R616, R617, R622, R623, R624, R625, R628, R629, R630, R632, R633, R634, R635, R636, R637, R638, R639, R640, R642, R643, R644, R645, R646, R648, R649, R650, R651, R652, R653, R654, R655, R656, R657, R658, R659, R660, R662, R663, R664, R665, R666, R667, R668, R669, R670, R672, R674, R675, R676, R677, R679, R680, R681, R682, R683, R684, R686, R687, R688, R689, R690, R692, R693, R694, R695, R696, R697, R698, R699, R700, R701, R702, R703, R704, R705, R706, R710, R711, R712, R714, R715, |

R717, R718, R720, R721, R722, R723, R724, R727, R728, R733, R734, R735, R736, R737, R738, R739, R740, R741, R742, R743, R744, R749, R750, R751, R752, R763, R764, R765, R766, R767, R768, R769, R770, R771, R772, R773, R774, R775, R776, R777, R778, R779, R780, R781, R782, R783, R784, R785, R786, R787, R788, R789, R790, R791, R792, R793, R794, R795, R796, R797, R798, R799, R800, R801, R802, R803, R804, R805, R806, R807, R808, R809, R810, R811, R812, R813, R814, R815, R816, R817, R818, R819, R820, R821, R822, R823, R824, R825, R826, R827, R828, R829, R830, R831, R832, R833, R834, R835, R836, R837, R838, R839, R840, R841, R842, R843, R844, R845, R846, R847, R848, R849, R850, R851, R852, R853, R854, R855, R856, R857, R858, R859, R860, R861, R862, R863, R864, R865, R866, R867, R868, R869, R870, R871, R872, R873, R874, R875, R876, R877, R878, R879, R880, R881, R882, R883, R884, R885, R886, R887, R888, R889, R890, R891

**Supplementary Table 6.** List of 162 essential reactions predicted under arbitrary complex medium.

| Reaction number of essential enzymes   |
|--|
| R001, R005, R006, R030, R031, R033, R035, R036, R044, R045, R046, R049, R050, R055, R056, R057, R058, R062, R063, R066, R068, R069, R070, R071, R095, R108, R143, R162, R163, R164, R165, R167, R169, R171, R172, R174, R175, R176, R177, R178, R179, R183, R184, R185, R186, R187, R188, R189, R190, R191, R192, R203, R227, R231, R232, R234, R235, R237, R238, R239, R244, R255, R256, R258, R278, R279, R282, R305, R309, R310, R311, R312, R313, R314, R316, R320, R328, R329, R331, R364, R381, R428, R431, R432, R433, R434, R523, R524, R525, R526, R527, R528, R529, R571, R572, R593, R608, R609, R610, R612, R613, R614, R615, R616, R617, R618, R619, R620, R621, R622, R632, R633, R634, R635, R636, R637, R638, R639, R640, R642, R643, R644, R646, R647, R648, R649, R651, R655, R656, R662, R665, R672, R673, R674, R675, R678, R679, R680, R681, R688, R690, R692, R693, R696, R737, R745, R746, R747, R748, R749, R750, R753, R754, R755, R756, R757, R758, R759, R760, R761, R789, R796 |

**Supplementary Table 7.** List of 211 essential metabolites predicted under arbitrary complex medium. Full name of each essential metabolite is available in Supplementary Table 2.

| Filtering criteria   | Essential metabolites  |
|--|--|
| Final 9 candidates selected from filtering framework   | AHHMP, DGLU, DHDP, DHP, DHSK, DX5P, DQT, KDO, PABA   |
| Association with enzymes homologous to human proteome (13 essential metabolites removed)           | ASPSA, C120OH, C140OH, C171ACP, CHOR, DMK, MDAPIM, MK, MKH2, OPP, PHT, PPAACP, SME   |
| Presence in human metabolism (75 essential metabolites removed)                                    | ACACP, ACCOA, ACP, AHTD, ARG, ASN, ASP, bALA, bDGLC, C100ACP, C120ACP, C140ACP, C150ACP, C160ACP, C161ACP, C170ACP, C180ACP, C181ACP, CDPDG, CYS, DADP, DALA, DCDP, DCTP, DGDP, DGTP, DHAP, DHF, DTDP, DTDPLU, DTDPRMNS, DTMP, DTTP, DUMP, E4P, F6P, FDP, FMN, G1P, G3P, G6P, GL3P, GLC, GLY, HCO3, HIS, ILE, LEU, LYS, MALACP, MET, NAAD, NACN, OBUT, OIVAL, PE, PEP, PG, PHE, PL, PPACOA, PRO, PRPP, PS, R5P, RL5P, SER, SUCCOA, THR, TRP, TYR, UDPG, UDPNAG, VAL, XMP   |
| Association with less than 3 reactions or 2 consuming reactions (82 essential metabolites removed) | 2AG3PE, 3A2OP, 3DDAH7P, 3PSME, 4PPNCYS, 4PPNTE, 4PPNTO, 5MC, A5P, A6RP, A6RP5P, A6RP5P2, ADCHOR, AGL3P, ALAALA, ASUC, CAV, CL, D6RP5P, D8RL, DAPIM, DATP, DB4P, DHN, DHPANT, DHPT, DNA, DPCOA, DT, DTDP4O6DG, DTDP4ORMNS, ER4P, EXOPOLYS, GA1P, GA6P, GDPMAN, IASP, ICHOR, KDOP, LIPID, LPS, MALCOA, MAN1P, MAN6P, NAGA1P, OHB, OSB, OSBCOA, P5P, PA, PANT, PEPTIDO, PGP, PHOSPHOLIPID, PL5P, PNTD, PPEPTIDO, PROTEIN, PYRDX, QA, RIBFLAV, RNA, SAOPIM, SDAPIM, SHCHC, SME3P, TDHDP, TM, UDCP, UDCPP, UDPAGLACA, UDPGAL, UDPMNLADGMD, UDPMNLADGMDDADA, UDPNAGEP, UDPNAM, UDPNAMA, UDPNAMAG, UPPMN(GN)LADGMDDADA, UPPMN(GN)LADGNMD(G)5DADA, UPPMN(GN)LADGNMDDADA, UPPMNLADGMDDADA |
| Currency metabolites (32 essential metabolites removed)  | ADP, AKG, ALA, AMP, ATP, CDP, CO2, COA, CTP, FAD, GDP, GLN, GLU, GMP, GTP, H2O2, IMP, METTHF, NAD, NADP, NADPH, NH3, O2, OTHIO, PI, PYR, RTHIO, SAM, THF, UDP, UMP, UTP  |