**Table S1. New metabolites added to *i*GC535**

|  |  |
| --- | --- |
| **Metabolite** | **Metabolite Name** |
| 1nphtol | 1-Naphthol |
| 2a3o4pob | 2-Amino-3-oxo-4-phosphonooxybutyrate |
| 2nphtol | 2-Naphthol |
| benz | Benzene |
| chlben | Chlorobenzene |
| chlphenol | 4-Chlorophenol |
| cyt552moxi | Membrane Cytochrome c522 oxidized |
| cyt552mred | Membrane Cytochrome c522 reduced |
| cyt552oxi | Cytochrome c552 oxidized |
| cyt552red | Cytochrome c552 reduced |
| cyt554oxi | Cytochrome c554 oxidized |
| cyt554red | Cytochrome c554 reduced |

**Table S2. New reactions added to *i*GC535**

|  |  |  |
| --- | --- | --- |
| **Reaction** | **Reaction Name** | **Stoichiometric equation** |
| AMO\_Np | Ammonia monooxygenase | o2\_p + 2 h\_c + q8h2\_c + nh4\_p -> h2o\_p + q8\_c + 3 h\_p + ham\_p |
| HAO | Hydroxylamine oxidase | h2o\_p + 4 cyt554oxi\_p + ham\_p -> 5 h\_p + 4 cyt554red\_p + no2\_p |
| NOOxi | Nitric oxide oxidase | h2o\_p + no\_p + cyt554oxi\_p -> 2 h\_p + cyt554red\_p + no2\_p |
| CoDen2 | CoDenitrification | h\_c + no2\_c + ham\_c -> 2 h2o\_c + n2o\_c |
| HAMtpp | Hydroxylamine transport (diffusion) | ham\_c <=> ham\_p |
| HAMtex | Hydroxylamine transport via diffusion (extracellular to periplasm) | ham\_e <=> ham\_p |
| UAAGMDtex | Uaagmda transport (periplasm) | uaagmda\_e <=> uaagmda\_p |
| UAAGMDtpp | Uaagmda transport (periplasm) | uaagmda\_p <=> uaagmda\_c |
| PDX5PSa | Pyrodoxine-5-phosphate synthase a | nad\_c + phthr\_c -> h\_c + nadh\_c + 2a3o4pob\_c |
| ADENOSINEase | ADENOSYL HOMOCYSTEINASE | ahcys\_c + h2o\_c -> hcys\_\_L\_c + adn\_c |
| METAOXIGENASE | Methane oxidation | o2\_p + q8h2\_c + ch4\_p -> h2o\_p + q8\_c + meoh\_p |
| EX\_benz\_e | Benzene Exchange | benz\_e -> |
| BENZtex | Benzene transport via diffusion extracellular to periplasm | benz\_e <=> benz\_p |
| BENZOXI2 | Benzene oxidation | o2\_p + q8h2\_c + benz\_p -> h2o\_p + q8\_c + phenol\_p |
| PHENOLOXI | Phenol oxidation | o2\_p + q8h2\_c + phenol\_p -> h2o\_p + q8\_c + hqn\_p |
| HYDROQUINONEtex | Hydroquinone transport via diffusion (extra-organism to periplasm) | hqn\_p <=> hqn\_e |
| XMO2 | Toluene monooxygenase | o2\_p + q8h2\_c + tol\_p -> h2o\_p + q8\_c + bzalc\_p |
| BZALDHMono | Benzyl alcohol dehydrogenase amo | o2\_p + q8h2\_c + bzalc\_p -> 2 h2o\_p + q8\_c + bzal\_p |
| EX\_chlben\_e | Chlorobenzene exchange | chlben\_e -> |
| CHLBENtex | Chlorobenzene transport via diffusion (extracellular to periplasm) | chlben\_e <=> chlben\_p |
| chlbenOXI | Chlorobenzene oxidation | o2\_p + q8h2\_c + chlben\_p -> h2o\_p + q8\_c + chlphenol\_p |
| CHLPHENOLtex | Chlorophenol transport via diffusion (extracellular to periplasm) | chlphenol\_e <=> chlphenol\_p |
| EX\_chlphenol\_e | 4-Chlorophenol exchange | chlphenol\_e <=> |
| CYT552OXI | Cytochrome c552 oxidase | 0.5 o2\_c + 4 h\_c + 2 cyt552red\_p -> h2o\_c + 2 h\_p + 2 cyt552oxi\_p |
| NITRRED | Dissimilatory nitrite reductase (NO-forming) | 2 h\_p + no2\_p + cyt552red\_p -> h2o\_p + no\_p + cyt552oxi\_p |
| NORED2 | Nitric Oxide Reductase | 2 h\_p + 2 no\_p + 2 cyt552red\_p -> h2o\_p + n2o\_p + 2 cyt552oxi\_p |
| CYTbc1 | CytCbc1 reductase using ubiquinol-8 | q8h2\_c + 2 cyt552oxi\_p -> q8\_c + 2 h\_p + 2 cyt552red\_p |
| Q8H2ASE | Ubiquinol Synthase | q8\_c + 2 h\_p + 2 cyt552mred\_c -> q8h2\_c + 2 cyt552moxi\_c |
| CYTEX | Cytochrome exchange | cyt554red\_p + cyt552moxi\_c -> cyt554oxi\_p + cyt552mred\_c |
| CYTPER | Cytochrome c552 peroxidase Nitrosomonas | 2 h\_p + h2o2\_p + 2 cyt552red\_p -> 2 h2o\_p + 2 cyt552oxi\_p |