*Ligilactobacillus murinus* Protocol

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| Model Version | Object (Type) | ID | Change | Impact | Notes |
| 1.1.1 | Metabolites  Reactions | cpd17041\_e0  cpd17042\_e0  cpd17043\_e0  EX\_cpd17041\_e0  EX\_cpd17042\_e0  EX\_cpd17043\_e0  SK\_cpd17041\_c0  SK\_cpd17042\_c0  SK\_cpd17043\_c0 | Metabolites:   * ID   Reactions:   * Eliminated * Created | cpd17041\_c0  cpd17042\_c0  cpd17043\_c0 | The metabolites represent non-metabolic associated reactions:   * cpd17041\_e0 🡪 DNA Replication * cpd17042\_e0 🡪 RNA Replication * cpd17043\_e0 🡪 Protein-biosynthesis   Therefore, the assigned reactions were boundary reactions. However, since these reactions happen within the cell, they should be considered sink reactions and not exchange. Red reactions were eliminated, green reactions were created. |
| 1.1.2 | Metabolites | cpd00158\_e0  cpd03198\_e0  cpd00222\_e0  cpd00367\_e0  cpd03047\_e0  cpd00047\_e0 | Metabolites:   * Name | CELB-e0  Melibiose-e0  GLCN-e0  Cytidine-e0  Taurocholate-e0  Formate-e0 | All names of the mentioned metabolites had an extra “e0” added to their name. This was corrected. Now the metabolites’ name follows: (name)-e0 |
| 1.1.3 | Metabolite  Reaction | DM\_cpd01042\_c0  cpd01042\_c0 | Metabolite:   * Eliminate   Reaction:   * Eliminate | eliminated | Reaction and metabolite were associated to “sink for p\_cresol”. |
| 1.1.4 | Metabolites | cpd17041\_e0  cpd17042\_e0  cpd17043\_e0 | Metabolites:   * Changed compartment | Metabolites now in “c0” compartment | Now the metabolites for DNA Replication, RNA Replication and Protein-biosynthesis are in the “c0” (cytosol) compartment. |
| 1.1.5 | Reactions | EX\_cpd00158\_e0 -> CELB-e0-e0 Exchange  EX\_cpd03198\_e0 -> Melibiose-e0-e0 Exchange  EX\_cpd00222\_e0 -> GLCN-e0-e0 Exchange  EX\_cpd00367\_e0 -> Cytidine-e0-e0 Exchange  EX\_cpd03047\_e0 -> Taurocholate-e0-e0 Exchange  EX\_cpd00047\_e0 -> Formate-e0-e0 Exchange | Reactions:   * Name changed | EX\_cpd00158\_e0 -> CELB-e0 Exchange  EX\_cpd03198\_e0 -> Melibiose-e0 Exchange  EX\_cpd00222\_e0 -> GLCN-e0 Exchange  EX\_cpd00367\_e0 -> Cytidine-e0 Exchange  EX\_cpd03047\_e0 -> Taurocholate-e0 Exchange  EX\_cpd00047\_e0 -> Formate-e0 Exchange | Noticed that the reactions associated to the metabolites changed in version 1.1.2 also had the problem with their associated reactions´ name. The name of those exchange reactions was changed to the correct structure. |
| 2.1.1 | Model |  | The model was changed. |  | The previous model was a first reconstructed by gapseq using another media. The new draft model seems to have fewer orphan metabolites and reactions. The naming of several metabolites and reactions seems to be correct. |
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| 2.2.1 | Transport Reaction Bounds | To see the full list of changed reactions, check dataframe under pickles folder “2.1.1.pkl” | All exchange reactions identified having a specific influx amount (negative value in lower bound) were identified. That boundary value was set in most cases as the upper bound of the corresponding transport reactions. | Now transport reactions associated to those exchange reactions are responsible to constrain the influx of metabolites | This decision was taken to work with the boundary values of exchange reactions more freely without loosing the values previously set by gapseq. The 4 things that were avoided in this process were metabolites H+, H2O and Na+ as they are involved with a high number of reactions and thus would overwrite other bounds already set by other metabolites. Reaction rxn13392\_c0 was avoided because of its inverted bounds (-1000, 0). |
| 2.2.2 | Exchange Reaction Bounds | All exchange reactions | All exchange reactions bounds have been set to either (-1000,1000) or (0,1000) depending or their previous reversibility | Now the previous version data is stored in transport reactions only | This just sets everything to the standard binary values. |
| 2.2.3 | Thymidine e0 | cpd00184\_e0  EX\_cpd00184\_e0  rxn10892\_c0 | Added thymidine as an external metabolite, its exchange reaction and transport reaction. | Now Thymidine can carry flux and be consumed/secreted | The decision to add the transport reaction was done by comparing to cytidine. The transport reaction was taken from ModelSEED and added to the model |
| 2.2.4 | Cytidine | EX\_cpd00367\_e0 | Added exchange reaction for external cytidine | Now Cytidine can carry flux and be consumed / secreted | This was discovered along with adding Thymidine. |
| 2.2.5 | Palatinose | cpd01200\_c0  cpd01200\_e0  rxn05629\_c0  EX\_cpd01200\_e0  rxn13126\_c0 | Added the necessary reactions to add palatinose to the metabolic pathway | Now palatinose is a viable metabolite to add to media compound list | This was corrected by BioCyc under a certain Enzyme Classification assigned to an enzyme found in L. Murinus. |
| 2.2.6 | Transport Reactions | All transport reactions | Reverted the constraint bounds set for transport reactions after discussing with Ömer | Now all transport reactions are reassigned to the binary system (-1000, 0 or 1000) | I asked again because Pia would maybe have to deal with the same and he now listened and said that wasn´t biologic... |
| 2.2.7 | rxn13126\_c0 | Palatinose consuming reaction | Changed boundaries from (-1000,1000) to (0,1000) | Now the reaction is irreversible | This is now result in palatinose not being produced and be consequence secreted into the media |
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