**Methods**

**Adding annotations**

**Metabolites and Reactions:** Initially, the PA14 model did not contain any annotations for metabolites, reactions, or genes. ModelPolisher can be used to annotate metabolites and reactions of a metabolic model. To do so, identifiers of the BiGG database (BiGG-IDs) are required as metabolite or reaction identifiers, respectively. Since the identifiers of the model were obtained from the ModelSEED database, BiGG-IDs needed to be determined. For each metabolite, the BiGG-IDs was assessed manually. Since this is a very time-consuming procedure, the BiGG-IDs for the reactions were resolved in a semi-automated way: The cross-references of the ModelSEED database to other databases, such as BiGG or KEGG, were used to automatically obtain the BiGG-IDs for the respective ModelSEED reaction identifier. If more than one BiGG-ID was returned, the correct identifier was determined by manual inspection of the respective reaction. The BiGG-IDs of the metabolites and reactions were added as biological qualifier (‘BQB\_IS’) annotations to the model using libSBML Version 5.17.0. The annotations were added in accordance with the MIRIAM guidelines. After adding the BiGG-IDs to the model, the ModelPolisher was used for further annotations of the model’s reactions and metabolites for references to other databases, such as KEGG, MetaNetX, or MetaCyc. The recently published version of the ModelPolisher is now also able to use other database identifiers.

For the reactions, the obtained KEGG annotations were used to further add all pathways that are associated with the respective reaction to the model. The pathways were obtained using the KEGG-ID and KEGG API to request all associated pathways. The pathways were then added to the respective reactions using the biological qualifier ‘BQB\_OCCURS\_IN’ in libSBML.

**Genes:** The identifiers of the model genes were from the KEGG database. With the help of libSBML, the KEGG gene annotation was added to the model. For further gene annotations, the KEGG API was again used to request NCBI Protein IDs and Uniprot IDs, which were subsequently added as respective annotations to the model. Additionally, the ID mapper from PATRIC was used to request gene RefSeq and NCBI gene identifier, as well as identifiers of the ASAP database.

**SBO-Terms:** Systems Biology Ontology (SBO) terms can give semantic information or is used for annotation purposes. In our model, all genes were labelled as genes with the SBO-term ‘SBO:0000243’. All metabolites without a valid SBO-term were labelled as simple chemicals with the SBO-term ‘SBO:0000247’. Transport reactions were divided into (1) active transport, if ATP is required for the respective transport reaction (SBO:0000657), (2) passive transport, if no external energy is required (SBO:0000658), (3) symporter-mediated transport, if two or more molecules are transported into the same relative direction across a membrane (SBO:0000659), or (4) antiporter-mediated transport, if two or more molecules are transported in relative opposite directions across a membrane (SBO:0000660).

All metabolic reactions were labelled as biochemical reactions with the SBO-term SBO:0000176.

Upgrading SBML version

The initial PA14 model was represented in SBML Level 2 Version 1. The model was updated to the latest SBML edition, which is Level 3. With the help of libSBML, both the fbc-plugin and the groups-plugin were enabled.

**Fbc-plugin**: Initially, the chemical formulas and charges of the metabolites were stored in the notes field. With the fbc-plugin, the charges were added as features of the metabolites to the model. The fbc-plugin also enables the addition of gene products to the model.

**Groups-plugin:** In the initial model, the subsystems of the reactions were saved in the notes field. With libSBML and the groups-plugin, the subsystems were extracted from the notes field and added as groups to the model. For each subsystem, a list of reactions associated with that pathway according to the notes was created and added to the subsystem as members.

**Correcting charge and mass imbalances**

A list of all mass- and charge-imbalanced reactions was extracted from the model. From this list, all exchange, sink, demand and biomass reactions were excluded. Each remaining reaction was manually checked by looking up the reaction-ID in ModelSEED: (1) If the reaction status in ModelSEED was balanced (‘OK’), but differed from the reaction equation in the model, the model reaction was adapted according to ModelSEED and again checked for imbalances. (2) If the reaction in ModelSEED also has an imbalanced reaction status, other databases like MetaCyc, BiGG or KEGG were browsed and the model reactions were adapted according to the respective reactions in the external databases. Where required, chemical formulas, charges, coefficients were corrected, or chemical compounds were added or subtracted from the reactions according to the respective database reaction. All changed reactions are listed in Table X - Supplements

Assessing the quality of the reconstruction with memote

Memote is an open-source software that provides a measure for model quality.

Every change and improvement of the model was continuously documented and quality-assessed using memote Version 0.9.11.