

Fungal Model Construction in KBase

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<http://kbase.us>

Project Goals: The DOE Systems Biology Knowledgebase (KBase) is a free, open-source software and data platform that enables researchers to collaboratively generate, test, compare, and share hypotheses about biological functions; analyze their own data along with public and collaborator data; and combine experimental evidence and conclusions to model plant and microbial physiology and community dynamics. KBase’s analytical capabilities currently include (meta)genome assembly, annotation, comparative genomics, transcriptomics, and metabolic modeling. Its web-based user interface supports building, sharing, and publishing reproducible, annotated analysis workflows with integrated data. Additionally, KBase has a software development kit that enables the community to add functionality to the system.

Fungal genome-scale metabolic models are an efficient way of predicting phenotypes across various environmental conditions. However, automating the construction of high-quality fungal models has been a challenge. Here we introduce a methodology to construct genome-scale fungal models in an automated fashion based on a curated set of reactions that are derived from published fungal metabolic models. As the basis for the method, we have produced a fungal model template that encompasses the biochemistry data from these published models and the structural annotations from the related genomes (Fig. 1).

The methodology uses structural annotations of any user-submitted fungal genome and computes a set of orthologous proteins against the curated fungal template in order to assert the presence or absence of specific biochemical reactions and pathways. Once the orthologous protein families are determined, the related biochemistry data is propagated to construct a new draft metabolic model (Fig. 1). In addition, useful statistical data that was generated during the model construction process is presented as part of the method output report (Fig. 2a, Fig. 2b). This method is deployed in KBase as an app (currently still in beta) called “Build Fungal Model”. The draft model that is generated by this app can be used for further analyses by utilizing a number of modeling related apps that are available in KBase.

Figure 1.

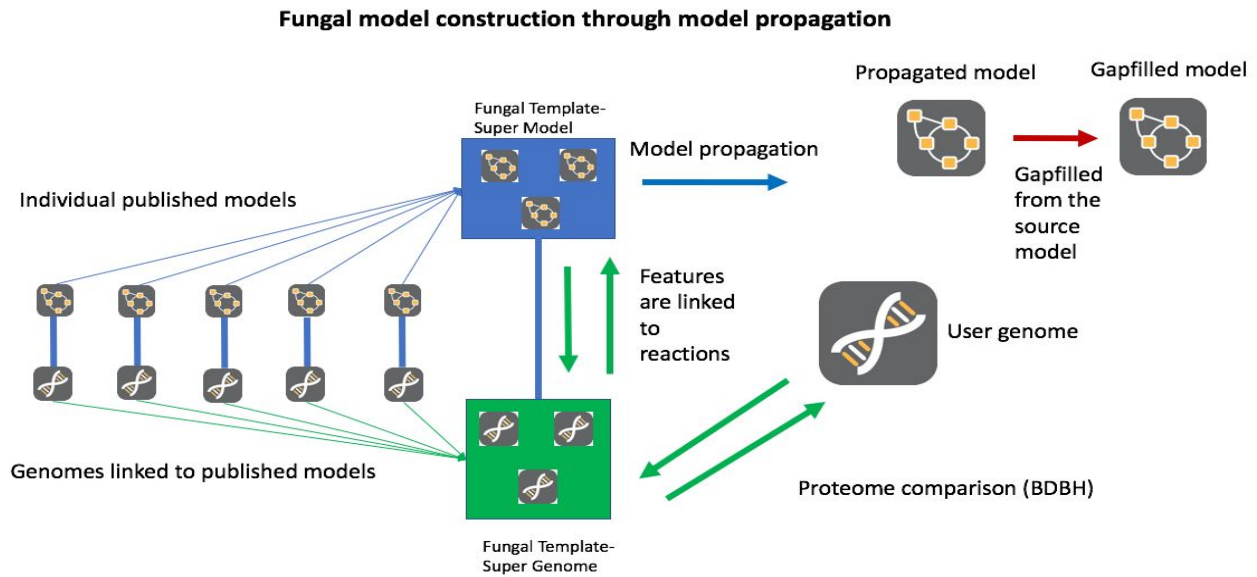


Figure 2a.

Published Model Intergregation Statistics

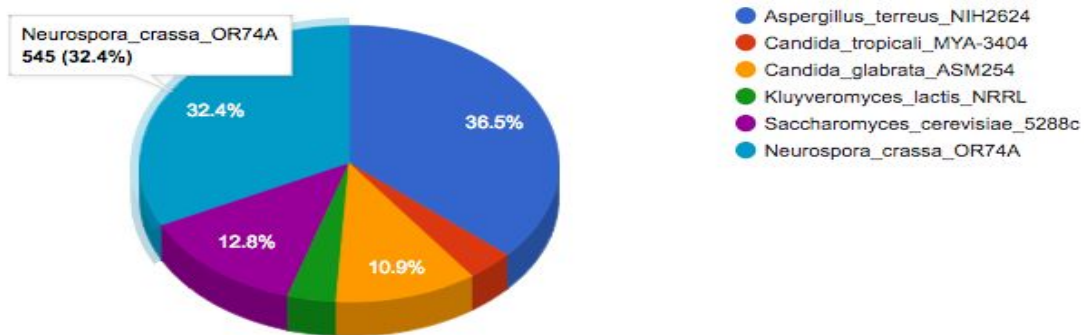
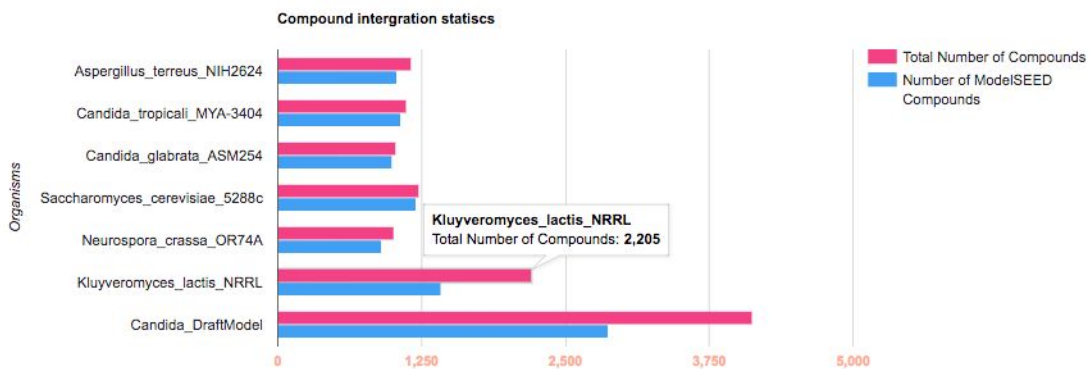


Figure 2b.



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