Modelling interspecies interactions of syntrophic communities

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Microbial communities have gained special interest by reconstructing models for practical applications such as biorefineries, bioelectricity generation and bioremediation. However, studying these communities has proven to be difficult due to the absence of experimental protocols and computational tools like the ones available for single organism. Using the genome annotations of two mutualistic species, single species modelling protocols can be adapted to microbial communities and the resulting microbial community genome-scale model will allow identifying several types of possible metabolic interactions between the two microorganisms. Hence, the main objective of this project is to develop a microbial community genome-scale metabolic model of syntrophic communities of anaerobic bacteria and archaea, namely *Desulfovibrio vulgaris* Hildenborough and *Methanococcus maripaludis* S2. For this purpose, models for both species will be integrated integrated into a single consortium model.

Focusing on reconstructing *Desulfovibrio vulgaris* Hildenborough model, the *merlin* framework [1], developed in-house, will be used to perform all steps of the reconstruction process. Initially, this process starts by uploading the genome annotation from UniProt and into *merlin's* database. *merlin* is a user-friendly Java application that performs the reconstruction of genome-scale metabolic models for any organism that has its genome sequenced. It performs the major steps of the reconstruction process, including the functional genomic annotation of the whole genome and subsequent collection of the portfolio of reactions. The reconstruction process involves identifying metabolic reactions, verifying the stoichiometry of the reactions, confirming the localization of the reactions, assembling the biomass equation and including it in the model together with other constrains. This process is constantly being refined by identifying and removing pathway dead ends, creating drains and enriching the composition of other metabolites, such as e-lipids, based on literature. Regarding the second organism, the *M. maripaludis* genome-scale metabolic model was previously published by another group [2].

Lastly, the *D. vulgaris* and *M. maripaludis* genome-scale metabolic models will be merged and *OptCom,* which is a comprehensive flux balance analysis framework for microbial communities, will be used to test and validate the above results from the organisms' metabolic interaction *in silico*. The availability of this framework besides *merlin* is a great addition to facilitate working process and obtain more accurate results.

References

[1] O. Dias, M. Rocha, E. C. Ferreira, and I. Rocha, "Reconstructing genome-scale metabolic models with merlin," Nucleic Acids Res., vol. 43, no. 8, pp. 3899–3910, Apr. 2015.

[2] Zomorrodi, A. R., & Maranas, C. D. (2012). OptCom: A Multi-Level Optimization Framework for the Metabolic Modeling and Analysis of Microbial Communities. PLOS Computational Biology, 8(2), e1002363. Retrieved from https://doi.org/10.1371/journal.pcbi.1002363