

Title

Continuous Validation Environment of the Metabolic Models of 5 Bacteria Organisms for the Production of Calcium Carbonate

Authors

Victor Emmanuel Rodriguez Torres^{1,2}, Jeremy Zucker², Andrew McNaughton², Tesia Lin²

¹Bioinformatics Science Program, The University of Texas at El Paso, El Paso, TX.

²Systems Biology Department, Pacific Northwest National Laboratory, Richland, WA.

Abstract

The Systems Biology Department at Pacific Northwest National Laboratory (PNNL) focuses on the study of microbial interactions and their potential applications in various environmental and biological processes. Within this group there is a project called Concerto-CarbStor which primary focus is utilizing metabolic modeling tools to explore cross-feeding interactions among 5 bacterial communities for enhanced calcium carbonate production. Python-based software such as Cobrapy, MICOM, and SMETANA to analyze community models and identify potential metabolic exchanges between organisms was used. Additionally, GitHub Actions and MEMOTE were integrated into the workflow to automate model quality assessments, allowing continuous improvement of metabolic models based on growth data experiments. Through SMETANA, community-wide metabolite interactions were computed, contributing to the understanding of metabolic dependencies within microbial consortia. The automated MEMOTE pipeline developed for five microbial models enabled continuous testing and validation of model improvements in GitHub. By doing a pull request, MEMOTE automatically generated three reports to calculate the quality of the metabolic models of the different 5 organisms, allowing PNNL researchers to easily calculate this metric after making a change in the metabolic model.