

A software package to assess the metabolic potential of mutant strains of the *Corynebacterium glutamicum*

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Motivation and Aim: In the bacterial biotechnology industry, the process of perspective strains searching is never ends. In this search, experimental approaches generate arrays of genomic, metabolomics and other types of data for many bacterial strains. Analysis of such data deals with approaches of bioinformatics, systems biology, mathematics and computational modeling. It allows one to propose a scheme of bacterial metabolic network functioning consistent with the observed data, and to suggest possible scenarios for biotechnological and/or genomic manipulations to optimize bacterial metabolism. In the study, we propose a semi-automated approach and its software implementation to analyze the evaluation of the metabolic potential of mutant strains and its validation on the example of *C.glutamicum* bacterial strains.

Methods and Algorithms: Software package is developed with programming language Python, and libraries cobraPy (cobrapy.readthedocs.io) and Pandas. Metabolic maps creation and visual interpretation of simulation experiments are performed with Escher tool (escher.readthedocs.io).

Results: To organize the computational flow for the analysis of mutation variants of the target strain, a software package was developed that implements a series of computational protocols. The computational protocols are presented in the form of Jupyter notebooks. This solution does not require a researcher to have a high level of proficiency in programming languages, and allows modifications of the work scenario if necessary. The program accepts a ready-to-use whole-genome flux model of bacteria in cobraPy format as input. The following functions are available: analysis of growth conditions on culture media; assessment of the potential of mutant strains. Implementations of these functions requires screening the parameters for hundreds of metabolic reactions within the computational experiment with further verification of acceptable solutions, which requires running the analysis on high-performance computing clusters.

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