## عنوان مقاله:

Inhibition of competitive pathways to increase butanetriol production in the Escherichia coli through metabolic network simulation

## محل انتشار:

یازدهمین همایش ملی و دومین همایش بین المللی بیوانفورماتیک ایران (سال: 1401)

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### خلاصه مقاله:

Supplying clean, renewable, and abundant energy is one of the main concerns of today's human civilization. Fossil fuels are limited and expensive, and damages caused by their use have made people turn to biofuels which are part of renewable energy. One of these valuable substances that can be obtained from microorganisms today with the advancement of metabolic engineering and bioinformatics is 1.Y.F-butanediol, an unnatural chemical substance with high value, and its properties are similar to glycerol. This chemical has essential applications as a precursor in manufacturing 1,Y,F-butanediol trinitrate as a product in the military industry, polymers, and medicines. In this study, the genome-scale metabolic network reconstruction of Escherichia coli (iML1@1@) was modeled for butanetriol production from the cheap carbon source, xylose. For this purpose, we applied the "Constraint-Based Reconstruction and Analysis" (COBRA) method by using the COBRA toolbox, an extension implemented in MATLAB software. The pathway for butanetriol production from xylose was optimized, and competing pathways that consumed xylose were blocked. The result of the FBA analysis showed that the reconstructed network for butanetriol production has flux. Hence, its output in the metabolic network of Escherichia coli was possible in silico. Finally, an attempt was made to determine the necessary and unnecessary reactions for improving butanetriol production by applying additional constraints and making some transcriptomics analysis. Considering that the complete deletion of competitive genes decreased the amount of biomass production by increasing the time required for proliferation; so by reducing the expression of competitive genes and not deletion, the amount of the butanetriol production reached YomMol/gDW/hr, which is a significant increment compared to the time of complete genes deletion.

**کلمات کلیدی:** Metabolic network modeling, ۱, ۲, ۴-butanetriol, E. coli , COBRA toolbox

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