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Title: Dynamic metabolic modeling of lipid accumulation and citric acid production by *Yarrowia lipolytica*

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<AT>Dynamic metabolic modeling of lipid accumulation and citric acid production by *Yarrowia lipolytica*

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- <ABS-Head><ABS-HEAD>Graphical abstract ► HIGHLIGHTS ► Development of three dynamic metabolic models for lipid accumulation. ► Modeling metabolic shifts of *Yarrowia lipolytica* for different cultures. ► Successful reproduction the experimental data by the models.

<ABS-HEAD>ABSTRACT

<ABS-P>*Yarrowia lipolytica* has the capacity to accumulate large amounts of lipids triggered by a depletion of nitrogen in excess of carbon source. However, under similar conditions this yeast also produces citric acid decreasing the lipid conversion yield. Three dynamic metabolic models are presented to describe lipid accumulation and citric acid production by *Yarrowia lipolytica*. First and second models were respectively based on the Hybrid Cybernetic Modeling (HCM) and the Macroscopic Bioreaction Modeling (MBM) approaches. The third model was a new approach based on the coupling between MBM and fuzzy sets. Simulation results of the three models fitted acceptably the experimental data sets for calibration and validation. However, MBM is time-dependent to consider metabolic shifts, and thus impractical for further applications. HCM and Fuzzy MBM adequately managed and described metabolic shifts presenting highlighting features for control and optimization. HCM and Fuzzy MBM were statistically compared reflecting similar results.

<KWD>Keywords: Dynamic metabolic modeling; Elementary modes (EMs); Hybrid Cybernetic Model (HCM); Macroscopic Bioreaction Model (MBM); Lipid accumulation; *Yarrowia lipolytica*;

<td:DefL>Nomenclature

<xps:span class=def>ATP</xps:span> <xps:span class=defd>Adenosine Triphosphate
[mol.mol⁻¹]</xps:span>

<xps:span class=def>*b*</xps:span> <xps:span class=defd>Fraction of catalytic biomass [-]
</xps:span>

<xps:span class=def>*C*</xps:span> <xps:span class=defd>Concentration of extracellular
metabolites [g.L⁻¹]</xps:span>

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