

# Development of computational and experimental methods for biomass composition and evaluation of its impact in genome-scale models prediction.

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The use of genome-scale metabolic models has been rapidly increasing in fields such as metabolic engineering. An important part of a metabolic model is the biomass equation since this reaction will ultimately determine the predictive capacity of the model in terms of essentiality and flux distributions. Thus, in order to obtain a reliable metabolic model the biomass precursors and their coefficients must be as precise as possible. Ideally, determination of the biomass composition would be performed experimentally, but when no experimental data are available this is established by approximation to closely related organisms. Computational methods however, can extract some information from the genome such as amino acid and nucleotide compositions.

The main objectives of this study were to compare the biomass composition of several organisms and to evaluate how biomass precursor coefficients affected the predictability of several genome-scale metabolic models by comparing predictions with experimental data in literature. For that, the biomass macromolecular composition was experimentally determined and the amino acid composition was both experimentally and computationally estimated for several organisms.

Sensitivity analysis studies were also performed with the *Escherichia coli* iAF1260 metabolic model concerning specific growth rates and flux distributions.

The results obtained suggest that the macromolecular composition is conserved among related organisms. Contrasting, experimental data for amino acid composition seem to have no similarities for related organisms. It was also observed that the impact of macromolecular composition on specific growth rates and flux distributions is larger than the impact of amino acid composition, even when data from closely related organisms are used.