BOFdat: Generating biomass objective functions for genome-scale metabolic models from experimental data - DTU Orbit (23/10/2019)

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Genome-scale metabolic models (GEMs) are mathematically structured knowledge bases of metabolism that provide phenotypic predictions from genomic information. GEM-guided predictions of growth phenotypes rely on the accurate definition of a biomass objective function (BOF) that is designed to include key cellular biomass components such as the major macromolecules (DNA, RNA, proteins), lipids, coenzymes, inorganic ions and species-specific components. Despite its importance, no standardized computational platform is currently available to generate species-specific biomass objective functions in a data-driven, unbiased fashion. To fill this gap in the metabolic modeling software ecosystem, we implemented BOFdat, a Python package for the definition of a Biomass Objective Function from experimental data. BOFdat has a modular implementation that divides the BOF definition process into three independent modules defined here as steps: 1) the coefficients for major macromolecules are calculated, 2) coenzymes and inorganic ions are identified and their stoichiometric coefficients estimated, 3) the remaining species-specific metabolic biomass precursors are algorithmically extracted in an unbiased way from experimental data. We used BOFdat to reconstruct the BOF of the Escherichia coli model iML1515, a gold standard in the field. The BOF generated by BOFdat resulted in the most concordant biomass composition, growth rate, and gene essentiality prediction accuracy when compared to other methods. Installation instructions for BOFdat are available in the documentation and the source code is available on GitHub (https://github.com/jclachance/BOFdat).

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