

Subject Section

RBAb: a pipeline to build genome-scale cellular models

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Associate Editor: XXXXXXXX

Received on XXXXX; revised on XXXXX; accepted on XXXXX

Abstract

Motivation: Yes

Results: No

Availability: The software is freely available and can be downloaded from

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Supplementary information: Supplementary data are available at *Bioinformatics* online.

1 Introduction

Parcimonious resource allocation emerged as a strong design principle for microorganisms (Goelzer *et al.*, 2009; Scott *et al.*, 2010). Based on this principle, new types of genome-scale cellular constraint-based models have been developed (Goelzer *et al.*, 2011; O'Brien *et al.*, 2013). In particular, we developed the resource balance analysis (RBA) method that has been recently validated for the bacterium *Bacillus subtilis* (Goelzer *et al.*, 2015).

RBA models integrate 3 set of constraints: mass balance in the metabolic network such as in genome-scale metabolic models (Varma and Palsson, 1994), capacity constraints on cellular processes and density constraints on the cytosol and membrane occupancy (reviewed in Goelzer and Fromion (2017)). RBA models necessitate various sources of information on cellular economics (composition of molecular entities, processing costs and composition of cellular processes, etc.) and quantitative parameters related to cell physiology or to the efficiency of molecular machineries (Goelzer and Fromion, 2017).

In this paper, we present a pipeline that builds a valid RBA model from an SBML file. Information about molecular composition is retrieved in a semi-automated process. The pipeline generates a model containing basic cell processes. The model is written in XML files to enable further enrichments.

2 Source of information

Resource allocation models require various sources of information.

Fig. 1. Caption, caption.

3 Pipeline structure

We present the *rba* Python package. *rba* was designed to perform three tasks.

- Build a working RBA model from an SBML file and Uniprot data. A RBA model can be exported to a set XML files (see Supplementary Material).
- Solve a RBA model.
- Visualize solutions.

4 Illustration

Illustration of prerba and nice output for subtilis/coli.

5 Conclusion

Acknowledgements

Funding

This work has been funded by the French Lidex-IMSV of the University Paris-Saclay.

Conflict of Interest: none declared.

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