SBOannotator: a Python tool for the automated assignment of systems biology ontology terms

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Abstract

Motivation

The number and size of computational models in biology have drastically increased over the past years and continue to grow. Modeled networks are becoming more complex, and reconstructing them from the beginning in an exchangeable and reproducible manner is challenging. Using precisely defined ontologies enables the encoding of field-specific knowledge and the association of disparate data types. In computational modeling, the medium for representing domain knowledge is the set of orthogonal structured controlled vocabularies named Systems Biology Ontology (SBO). The SBO terms enable modelers to explicitly define and describe model entities, including their roles and characteristics.

Results

Here, we present the first standalone tool that automatically assigns SBO terms to multiple entities of a given SBML model, named the SBOannotator. The main focus lies on the reactions, as the correct assignment of precise SBO annotations requires their extensive classification. Our implementation does not consider only top-level terms but examines the functionality of the underlying enzymes to allocate precise and highly specific ontology terms to biochemical reactions. Transport reactions are examined separately and are classified based on the mechanism of molecule transport. Pseudo-reactions that serve modeling purposes are given reasonable terms to distinguish between biomass production and the import or export of metabolites. Finally, other model entities, such as metabolites and genes, are annotated with appropriate terms. Including SBO annotations in the models will enhance the reproducibility, usability, and analysis of biochemical networks.

Availability and implementation

SBOannotator is freely available from https://github.com/draeger-lab/SBOannotator/.