SBML Level 3 package: Multistate, Multicomponent and Multicompartment Species, Version 1, Release 2

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Abstract

Rule-based modeling is an approach that permits constructing reaction networks based on the specification of rules for molecular interactions and transformations. These rules can encompass details such as the interacting sub-molecular domains (components) and the states such as phosphorylation and binding status of the involved components. Conceptually, fine-grained spatial information such as the locations of the molecular components relative to a membrane (e.g. whether a modeled molecular domain is embedded into the inner leaflet of the cellular plasma membrane) can also be provided. Through "wildcards" representing component states, entire families of molecule complexes sharing certain properties can be specified as patterns. This can significantly simplify the definition of models involving species with multiple components, multiple states, and multiple compartments. The SBML Level 3 *Multi* Package (Multistate, Multicomponent and Multicompartment Species Package for SBML Level 3) Version 1 extends the SBML Level 3 Version 1 *core* with the "type" concept in the Species and Compartment classes. Therefore, reaction rules may contain species that can be patterns and exist in multiple locations. Multiple software tools such as *Simmune* and *BioNetGen* support the SBML Level 3 *Multi* package that thus also becomes a medium for exchanging rule-based models. This document provides the specification for Release 2 of Version 1 of the SBML Level 3 *Multi* package. No design changes have been made to the description of models between Release 1 and Release 2; changes are restricted to the correction of errata and the addition of clarifications. All the completed example models in this specification have been validated by the validation rules of SBML Level 3 Version 1 core and SBML Level

3 Multi package Version 1 using the libSBML library.