



Research Project in Bioinformatics

Graphical Editor for Systems Biology Models

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1 Background

In diverse applications, computational modeling has demonstrated to be useful for a variety of areas, ranging from fundamental research over biotechnology to applications within the health sector. As in other sciences, reproducible findings are of the highest importance. Over the past two decades, the format SBML [2] has advanced to the *de facto* standard for encoding systems biology models that satisfies this need [6]. However, this XML-based format has never been intended to be written or read by human users directly. Instead, dedicated software libraries should take care of importing and exporting models in SBML format.

Particularly in the life sciences, spreadsheet-based representations of information are prevalent.

According to a recent questionnaire, many researchers desire to develop their models in user interfaces that present the information in table form. The format SBTAB [4] has been developed to be compatible with SBML.

ID	Name	ReactionFormula	ID	Name	Compartment	isConstant
R549	R549	ACETL_C6A + NADH <=> ACALD + NAD + C6ASH	ACETATE	acetate	Cell	false
R549b	R549b	ACALD + NADH <=> ETOH + NAD	ACETATE_ext	extracellular acetate	external	false
R151	R151	RIBOSE_5_P + XYL_5_P <=> XYL_3_P + GA_3P	ACETYL_C6A	acetyl-coenzyme A	Cell	false
R247	R247	SUCC_C6A + ADP <=> SUCC + ATP + C6ASH	ACALD	acetaldehyde	Cell	false
R157	R157	ERTH_4_P + XYL_5_P <=> GA_3P + FRU_6_P	ACETYL_P	acetyl phosphate	Cell	false
R96	R96	FORMATE <=> FORMATE_ext	ADP	adenosine diphosphate	Cell	false
R94	R94	ACETATE <=> ACETATE_ext	AMP	adenosine triphosphate	Cell	false
R95	R95	SUCC <=> SUCC_ext	ATP	adenosine triphosphate	Cell	false
R93	R93	ME3_ext <=> ME3	ATP_mash	maintenance energy	external	false
R90	R90	ETOH <=> ETOH_ext	BIOBIOMASS	biomass	external	false
R01	R01	ACETATE <=> ACETATE_ext	CITRATE	citrate	Cell	false
R87	R87	PG <=> PEP	CO2	carbon dioxide	Cell	false
R109	R109	GLU_6_P + NAD <=> GLU_LAC_6_P + NADH	CO2_ext	extracellular carbon dioxide	external	false
R108	R108	GLU_LAC_6_P <=> GLUCO_6_P	C6ASH	coenzyme A	Cell	false
R102	R102	GLUCO_6_P + NAD <=> FRIBULOSE_5_P + NADH + CO2	DNAP	dihydroxyacetone phosphate	Cell	false
R287	R287	FORMATE <=> MALATE	ERTH_2_P	erythrose-4-phosphate	Cell	false
R3	R3	FRU_6_P + ATP <=> FRU_BIS_5_P + ADP	ETOH	ethanol	Cell	false
R70	R70	4.0 GLU_6_P + 13.0 RIBOSE_5_P + 5.0 ERTH_4_P + 32.0 PEP + 38.0 PIR + 41.0 ACE	ETOH_ext	extracellular ethanol	external	false
R67	R67	GA_3P <=> DNAP	FORMATE	formate	Cell	false
R97	R97	CO2 <=> CO2_ext	FORMATE_ext	extracellular formate	external	false
R27	R27	GLU_6_P <=> FRU_6_P	FRU_6_P	fructose-6-phosphate	Cell	false
R55a	R55a	ACETYL_C6A <=> ACETYL_P + C6ASH	FRU_BIS_5_P	fructose bi-phosphate	Cell	false

Figure 1 | Display of systems biology models in form of a spreadsheet.

2 Aim

In this project, a graphical user interface should be developed that presents systems biology models in a form similar to SBTAB, and that allows the user to edit the information. The software should cover the core of SBML as well as the so-called FBC extension (Flux Balance Constraints) for representing constraint-based models [5]. It should be programmed in a way to also enable the addition of further extension packages or additional levels and versions of SBML.

3 Approach

In a preceding bachelor's thesis¹ and as part of a students' team project², two different versions of such a user interface have been developed. The SBMLSheets project is based on the InSilico framework³ that is based on OSGi technology and FXclipse. As such, SBMLSheets can be used in combination with further plugins for the InSilico framework, such as the simulation core [3]. It is, therefore, most standardized and well suited for further extension. For this reason, it is intended to finalize an initial version of SBMLSheets as the result of this project. Recon 3D [1] is a useful example model for testing the software.

4 Requirements

- (1) Experience in Java™ programming and JavaFX
- (2) fundamental understanding of biochemistry
- (3) interest in systems biology modeling
- (4) enthusiasm and a sense for detail

References

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¹ [🔗/RobertDeibel/SBMLSheets](#)

² [🔗/draeger-lab/SBTabEditor/](#)

³ [🔗/draeger-lab/insilico/](#)