BioModels Database

Model Curation

CellML workshop,
ABI, Auckland

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Branches of BioModels Database

• Curated
  • checked for MIRIAM compliance
  • curation figure added
  • model elements manually annotated
  • BioModels ID (BIOMDxxxx)

• Noncurated branch
  • only slightly altered by the curators
  • only publication and creation details added automatically and by curators
MIRIAM compliance for BioModels DB


model must:

- be correctly encoded in a standard format (valid SBML)
- contain link to a single reference description (peer reviewed for BioModelsDB)
- contain creator's contact details
- reflect the structure of the processes and formulas described in the reference publication
- be able to reproduce the results given in the reference publication
Non Curated Branch

- valid SBML
- not MIRIAM compliant
  - not kinetic models (eg. FBA, stoichiometric maps)
  - can not reproduce results
- MIRIAM compliant
  - models contain kinetics that we do not curate up to now (eg. boolean models) or parts are not encoded in SBML (eg. spatial information)
  - significant tailback due to insufficient time and workforce → will be moved into curated branch as soon as possible
Curation Guidelines

- read publication
- go through SBML model and compare all elements
  - where possible create reactions out of differential equations
  - add names to unnamed reactions, rules and events
  - add compartments and move species and parameters accordingly
- change names and IDs to correspond to article
- try to reproduce one or two key results of the reference publication and create curation result (figure or table)
- add notes
- move model to the curated branch for annotation and publication

if any problems occur contact submitter first and, if necessary, authors. All deviations from the publication have to be documented in the notes whenever the model’s SBML file is changed significantly, the curation results have to be redone.
submission → SBML consistency check → compare model with original publication → non curated branch

annotation → curated branch gets BIOMD ID still not public

curated branch public → compare simulation results with publication
submission → SBML consistency check → compare model with original publication → non curated branch

SBML, enter units, beautify and correct SBML, change IDs and names → compare simulation results with publication → curated branch gets BIOMD ID still not public → annotation → curated branch public
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SBML consistency check

compare model with original publication

beautify and correct SBML, enter units, change IDs and names

compare simulation results with publication

annotation gets BIOMD ID, still not public

contact: submitter, creator or finally authors

add notes of changes

non curated branch

curated branch public

curated branch

submission

manually correct SBML
Comment: The model reproduces figure 3A of the reference publication. The model was integrated and simulated using Copasi v4.5 (Build 30).
Curation

Problems:
• typos and errors in publications – both in model or results
• original models used in publication not available
• misleading diagrams or simplified kinetics in model/publication
• automatically generated SBML files can be hard to interpret

only few models stay in the curation pipeline:
• no publication info or never published
• large deviations from the model structure of the publication