Supplemental Information

Best Practices for Making Reproducible

Biochemical Models

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General-Purpose Reproducible Biochemical Modeling Checklist

Data aggregation:

☐ New data collection and experimental procedures are reproducible

    ☐ The experimental protocol is provided

    ☐ Conditions that deviate from the standard protocol are provided

    ☐ Measurement uncertainty is quantified

    ☐ A record of when the data was collected is provided

    ☐ A record of the individual or lab that produced the data is provided

☐ Data collected from databases and literature are curated and metadata are provided

    ☐ All manipulations applied to measurements are described and the original data is referenced (e.g. statistical analyses, normalization)

    ☐ Database and data source entries are provided

    ☐ Ownership of the original data is credited

Model construction:

☐ All species and parameter names are biologically-relevant and unambiguous

    ☐ Shortened identifiers used in the model description are linked to the full species or parameter name in a supplemental table

    ☐ The full species or parameter names follow standardized naming conventions

☐ All reactions are uniquely identified

☐ Model components are described in computer-readable tables and automatically imported by simulation study code

☐ If a model uses differential equations, then its biochemical reactions and differential equations are both reported

Parameter estimation:

☐ Software generated to perform parameter estimation is provided

☐ Confidence intervals are reported on estimated parameters

☐ Families of parameter values are reported for non-identifiable models, if there are a discrete number of possibilities

☐ Uncertainty quantification is performed

Simulation:

☐ All initial conditions and parameter values are provided for each published simulation experiment

    ☐ Well-documented tables of parameter values for each unique simulation experiment are provided with the publication

☐ All simulation experiments are fully defined (events listed, collection times and measurements specified, algorithms provided, simulator specified, etc.)

☐ Algorithms required for executing the simulation are reported

    ☐ Numerical integration algorithms are reported

- ☐ Stochastic algorithms are reported
- ☐ Random number generator algorithms are reported
- ☐ Other algorithms are reported (e.g. steady state methods)
- ☐ Stochastic simulations are repeated to generate a representative distribution of simulation results
    - ☐ Seeds are recorded for each simulation result, a method for obtaining the seeds is provided, or a method for generating a statistically-similar distribution of results is provided

Results storage:

- ☐ All data is provided in supplemental tables or computer-readable spreadsheets (e.g. HDF file)
    - ☐ Unprocessed results are provided
- ☐ All data is annotated for comprehension
- ☐ Source data and code to produce published figures is provided

Verification & validation:

- ☐ All custom modeling code is systematically verified
    - ☐ A program is written which checks that all model components and numerical methods exhibit expected behavior
- ☐ The model and associated simulation experiments are validated to assess biological relevance
- ☐ The model and associated simulation experiments are tested in an independent computing environment to ensure that the software is portable and reproducible

Documentation:

- ☐ All data and software used to construct the model are documented
- ☐ Installation and usage instructions are recorded for the model and associated software (e.g. as a README file)
- ☐ Design decisions and assumptions are recorded
    - ☐ The biological relevance of the modeling study, including mathematical descriptions, and any simplifying assumptions are justified
    - ☐ The biological system context is described
    - ☐ The environmental context is described
- ☐ The model and all associated programs for simulation, analysis, and verification and validation are explained through comments
- ☐ Figures visualize the model—all components and interactions—and the results of simulation experiments, include detailed figure legends

Packaging:

- ☐ All model artifacts are organized in a single archive
- ☐ The model archive contains sub-directories which are described, along with all model artifacts, in a manifest file

Dissemination:

- ☐ The modeling study is disseminated in a pre-print server (e.g. bioRxiv)
- ☐ The modeling study is published in a peer-reviewed journal
- ☐ The model and source code are available at a public repository or personal web site
    - ☐ A permissive license to use repository materials is provided