

An application framework for predictive modeling of biological processes

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ABSTRACT

Entering the post-genomic era, the recent increase in availability and variety of biological data has stimulated demand for modeling and simulation to help elucidate experimental findings. The mathematical expertise required for model building, however, has limited its wide-spread application.

Physiome Sciences is developing a modeling framework (In Silico Cell™) that includes tools for simulating signal transduction pathways and other physiological processes that occur in the complex cellular milieu. These tools have expert-user capabilities but are also designed for researchers with no mathematical modeling experience. While providing hypothesis testing and predictive capabilities, the resulting models importantly become the entry point for accessing relevant data. The tools thus provide a unified environment to filter information, analyze data, develop hypotheses, and create a shared knowledgebase.

Physiome Sciences' In Silico Cell™ technology is designed around four core themes:

- **Transparent** – Researchers can choose to build and simulate a model without encountering the underlying mathematical formalism, or to edit the mathematics and data directly.
- **Customizable** – Physiome Sciences provides the tools for the researcher to build an individual model within a general framework. The researcher may also import custom mathematics during model construction or simulation.

- **Expandable** – Models can be re-used as components to build more realistic, larger-scale models as new data are generated.
- **Flexible** – Models can interface with other applications and build on the user's existing computational infrastructure

This poster focuses on the use of In Silico Cell™ to construct, analyze, and interpret biochemical pathway data. In Silico Cell™ supports the hierarchical modeling of biological systems and the creation of detailed models from simple ones. This process is enabled through the CellML™ model language, an application of XML for describing biological processes at the cellular and sub-cellular level. CellML is being developed as an open standard in a collaborative effort between Physiome Sciences and the University of Auckland Bioengineering Research Group.

This poster will show how In Silico Cell's Pathway Editor allows the researcher to build and edit pathway diagrams, and also use network analysis tools to identify possible drug targets at critical points in a biochemical pathway. This feature is accomplished through a graphical user interface that automatically generates simulations and mathematics from pathway maps. The pathway and its individual components are linked to a database that can be referenced and updated by the researcher.

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