

Poster I-63

SIGPATH: Information Management for the Modeling of Cellular Networks

Campagne, Fabien¹, Neves, Susana³, Chang, Chun-wen², Skrabanek, Lucy^{1,2}, Ram, Prahlad T.³, Iyengar, Ravi³, Weinstein, Harel^{1,2}

¹Department of Physiology and Biophysics and Institute for Computational Biomedicine, Weill Medical College of Cornell University, New York, NY, USA; ²Department of Physiology and Biophysics, ³Department of Pharmacology and Biological Chemistry, Mount Sinai School of Medicine, New York, NY, USA

Computational analysis of complex protein networks and interactions within cells requires the ability to develop quantitative models and to numerically compute the properties and behavior of the networks. In addition to numerical solvers, information management systems are needed, wherein the quantitative data associated to its biological context can be stored, curated and reliably retrieved. We have focused on biochemical computation of cellular interaction networks and developed an information management system (IMS) that stores quantitative information on the cellular components and interactions, as well as the basic reactions that can be used to construct a pathway and eventually a large-scale network. This system is called *SigPath* and is made available on the internet (<http://www.sigpath.org>). Key features of our approach include: (i) the use of background information (e.g. names of the molecules, aliases, and accession codes) to ease data submission and link this quantitative database with other qualitative databases, (ii) a strategy for the management of information that can be refined over time by multiple users, (iii) the development of data representation to store both qualitative and quantitative information, (iv) features designed to assist end-users in assembling custom quantitative models from the information stored in the IMS. Currently, models assembled in *SigPath* can be automatically exported for computation in several computing environments such as JSim, Kinetikit/Genesis, Virtual Cell, Jarnac/JDesigner. As a test of the system, we have constructed the β -adrenergic receptor-Gs interactions and MAP-kinase pathways with *SigPath*, and exported the models to each of the supported computing environments; the results were identical to those obtained from control simulations with manually entered and submitted data. When appropriately populated, this IMS will support efficient large-scale quantitative studies of cell signaling networks and other cellular networks. The poster will present the general scheme of *SigPath* (including both the information management scheme and system architecture), and will illustrate its application to specific studies in cell signaling pathway modeling.

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