

## Preface

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# Workshop on “Storage and Annotation of Reaction Kinetics Data”, Villa Bosch in Heidelberg, May 21–23, 2007

Isabel Rojas and Ulrike Wittig

*Scientific Databases and Visualization Group, EML Research gGmbH, Heidelberg, Germany*  
E-mail: [isabel.rojas@eml-r.villa-bosch.de](mailto:isabel.rojas@eml-r.villa-bosch.de), [wittig@villa-bosch.de](mailto:wittig@villa-bosch.de)

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Systems biology aims at providing a dynamic view of the living cell, tissue, or organism, by combining experimental and theoretical methods. Advances in experimental methods in biochemistry are making possible an increasingly detailed analysis of cellular processes. However, in many cases the data resulting from these experiments cannot be mechanistically explained with the existing knowledge because of the complexity of the biochemical networks. Therefore computer-assisted modelling, simulation and other mathematical methods are used for an interpretation of experimental data.

Setting up mathematical models of biochemical networks is a complex task that requires both the mathematical and biochemical knowledge as well as information about the kinetics of the biochemical reactions participating in the modelled networks. The success of system biology projects depends heavily on the exchange of information from experimentalists to modellers and *vice versa*. Data from experiments (wet-lab or *in silico*) need to be made available and searchable in a comprehensive and if possible automatic manner.

The main motivation for this workshop has been to bring together researchers working on the generation, storage, integration, annotation and usage of kinetic data of biochemical reactions in the context of systems biology. It aims at coordinating efforts in the development of resources for reaction kinetics data, taking into account the needs from both the experimentalists' side as well as from the modellers' point of view. The workshop has been divided into the following sessions: “Kinetic data generation”, “Storage and Integration of Reaction Kinetics' Data”, “Annotating Reaction Kinetics' data” and “Usage and Exchange of Reaction Kinetics' data”.

Databases for systems biology are now emerging, containing, among other, information about existing models, kinetic parameter values, and the descriptions of the mechanisms of biochemical reactions. However, most of these databases are populated mainly from information found in scientific publications and not from data provided directly by the experimentalists. This implies huge delays between the generation of the data and their availability through the above mentioned databases. Thus the importance to bring together experimentalists, database developers and modellers in order to exchange ideas on how the information should be submitted, stored and made available. Another crucial aspect of systems

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biology that we aim to address in this workshop deals with providing the results from simulations and models to the experimentalist, in order to improve the understanding of their experiments or to design new ones.

This special issue includes a series of short articles submitted by invited speakers of the workshop. In conjunction the articles present some of the efforts being carried out in order to provide high quality data for the systems biology community, reflecting also the needs for the data to comply to certain formats and standards, and giving examples on how the feed-back between experimentally generated data and *in-silico* simulations can improve the understanding of biochemical processes and permit the design of new experiments.

We would like to thank the invited speakers for their interest and corporation, the EML Research gGmbH, the Klaus Tschira Foundation gGmbH and the German Research Council for their financial and administration support, and last but not least the Editors of In Silico Biology for accepting to create a special issue for this workshop.