

# COMPUTATIONAL SYSTEMS BIOLOGY



INNOVATION

ENGINEERING

OPTIMIZATION

## Solutions for Pharmaceutical Research and Development

From early discovery on, pharmaceutical R&D projects generate an enormous wealth of information complementing public knowledge about the targeted disease and therapy approach. A major challenge for improving R&D efficiency is the integral representation and interpretation of all information and its comprehensive exploitation for decision making. Computational Systems Biology offers a unique way of dealing with knowledge, information and assumptions underlying a drug development project.

The Computational Systems Biology experts at Bayer Technology Services provide expert services and powerful modeling tools designed to support the selection, optimization, and application of active compounds at all stages of the drug R&D process. Our technology helps to accelerate the development process, reduce the costs of preclinical and clinical studies and increase their overall chances of success.

### Modeling and Simulation Platform

We offer a unique software platform for physiologically based pharmacokinetic and -dynamic (PBPK/PD) as well as disease modeling along the whole drug research and development process.

### PBPK/PD Modeling

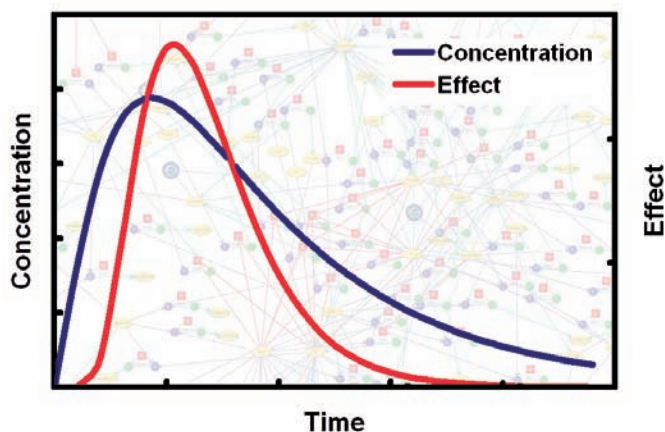
PK-Sim® and MoBi® are sophisticated tools for modeling pharmacokinetics (PK) and pharmacodynamics (PD), respectively, of active compounds in virtual human populations or animal species. The processes responsible for absorption, distribution, metabolism and excretion (ADME) in the body are simulated integrating physiological data (e.g. blood flows, organ volumes, tissue compositions etc.) representing state of the art knowledge and compound specific parameters. Compared to other pharmacokinetic modeling techniques, PBPK-modeling has a significantly lower demand for in vivo data with concomitantly higher predictive power when extrapolating to scenarios not covered by experimental data.

Drug effects in target organs depend on the local concentration of the respective compound. Therefore, coupling of PK-Sim® pharmacokinetic models describing the concentration-time course of a given drug with MoBi® pharmacodynamic models specifying drug exposure effects, offers the opportunity to predict drug response, optimize dose regimens, and decrease risk of clinical trial failure.

### Disease Modeling

Computational disease models help to analyze and understand complex diseases as relevant structural biological, physiological, medical, and pharmacological knowledge is summarized in one unified computational representation.

Established disease models support efficacy screening and proof-of-concept studies, verify efficacy of lead molecules and help to select compounds with therapeutic potential. Additionally, computational modeling supports the design of crucial validation experiments and assists in the extrapolation to following project steps.

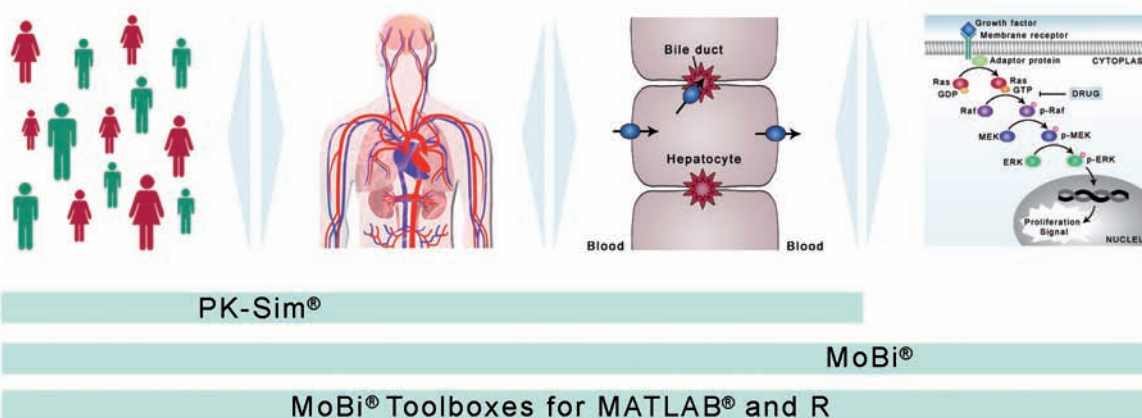


Concentration/Effect vs. time curves from PBPK/PD models



Bayer Technology Services  
Powering Your Performance

## Multiscale Modeling & Simulation of Pharmacokinetics, Pharmacodynamics and Disease Progression



Computational Systems Biology Modeling and Simulation Platform

### Software Solutions

All software products are fully integrated into one Computational Systems Biology Software Suite: a user-friendly and flexible software package for mechanistic modeling and simulation in pharmaceutical research and drug development.



#### PK-Sim®

The comprehensive software tool for whole-body physiologically based pharmacokinetic modeling.



#### MoBi®

The systems biology software tool for multiscale physiological modeling and simulation.



#### MoBi® Toolbox for MATLAB®

The advanced tool integrating multiscale physiological modeling and simulation with technical computing.



#### MoBi® Toolbox for R

The advanced tool integrating multiscale physiological modeling and simulation with statistical computing.



#### Customized Solutions

Tailor made software solutions to suit individual needs of customers.

Each software product can be used as a stand-alone solution for specific projects. The whole platform enables any complex modeling task with the MoBi® Toolboxes for MATLAB® and R. The software platform is open for integration of already existing open source and proprietary libraries and allows continuous extension of functionalities.

### Consulting Services

Our Computational Systems Biology experts conduct **complete application projects** from scope definition to reporting according to regulatory standards. In an independent analysis experimental data is integrated with information available from literature. Mechanistic models tailored to your specific problem are generated and applied for the simulation of scenarios that are of interest at any given stage of a R&D project.

We efficiently perform application projects in pharma research and life sciences relying on our unique software platform and our broad experience gained in hundreds of application projects accomplished in the following areas:

#### Drug Discovery Support

- Target Identification & Validation
- Biomarker Analysis
- Proof-of-Mechanism

#### Drug Development Support

- Species Extrapolation
- Extrapolation to Special Populations
- Proof-of-Concept
- Bioequivalence Studies

Additionally, we offer **customized trainings** to meet the needs of R&D scientists and PK experts working in the fields of drug development, clinical pharmacology and pharmacokinetics. In our opinion, providing tailored learning modules instead of generic training sessions ensures effective and appropriate use of our products and services.

For further information on our software tools and services visit our website [www.systems-biology.com](http://www.systems-biology.com) or write a message to [info@systems-biology.com](mailto:info@systems-biology.com).

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