



INNOVATION

ENGINEERING

OPTIMIZATION

The Systems Biology Software Tool for Multiscale Physiological Modeling and Simulation

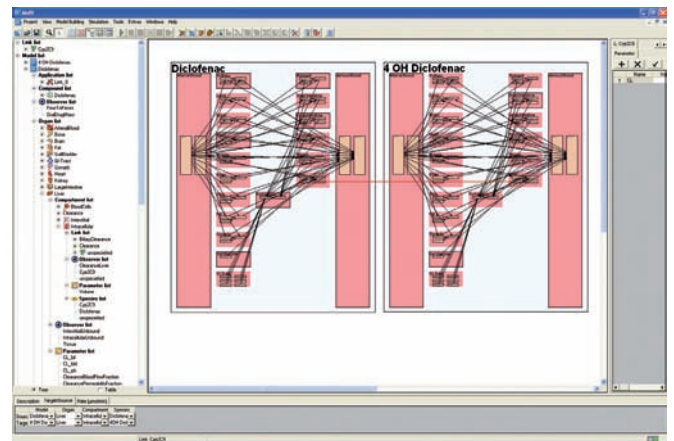
The increase in experimental data gained through advanced high-throughput experiments, genomics, proteomics and bioinformatics gives rise to unprecedented insights into biological mechanisms. Today's challenge is the integration of the available knowledge into a detailed quantitative description of a biological system and the underlying interacting processes.

Therefore, mechanistic modeling and simulation attracts more and more attention by scientists in drug research and development all over the world. Bayer Technology Services provides the software tools and consulting services that support these scientists to achieve their mission in a highly efficient way.

MoBi® is a sophisticated, flexible software package for mechanistic modeling of biological processes and drug actions. It is completely integrated with PK-Sim®, our package for physiologically-based pharmacokinetic (PBPK) modeling, and is, consequently, especially suitable for the analysis of complex pharmacokinetic and pharmacodynamic models under simultaneous consideration of whole-body physiology.

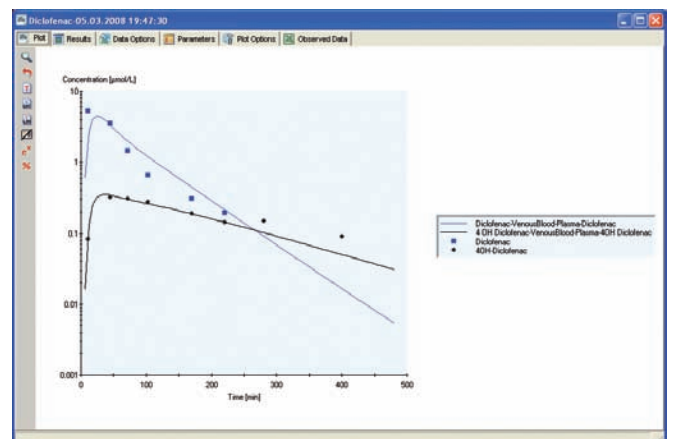
Modeling with MoBi® is a unique means to integrate in vitro and in vivo findings into one unified representation allowing for the evaluation, analysis, interpretation and prediction of experiments to an utmost level of detail.

MoBi® facilitates the processes of model building and simulation with its intuitive graphical user interface, the import and export to other modeling languages (e.g. SBML) and is a powerful visualization tool for simulation results. The integration of the recently developed MoBi® Toolboxes for MATLAB® and R allows for the seamless performance of complex optimizations and sensitivity analyses as well as the implementation of large simulation and analysis tasks that can be programmed to run automatically.



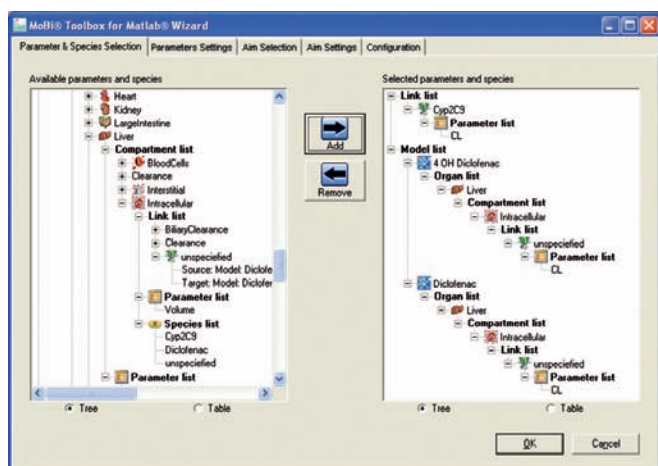
Integrating drug and metabolite models

Pharmacodynamic models in MoBi® can be easily integrated with pharmacokinetic simulations in PK-Sim®. Hence, the impact of different doses and dosing schedules can easily be investigated on a molecular level.



Comparing experimental data with simulated plasma concentrations

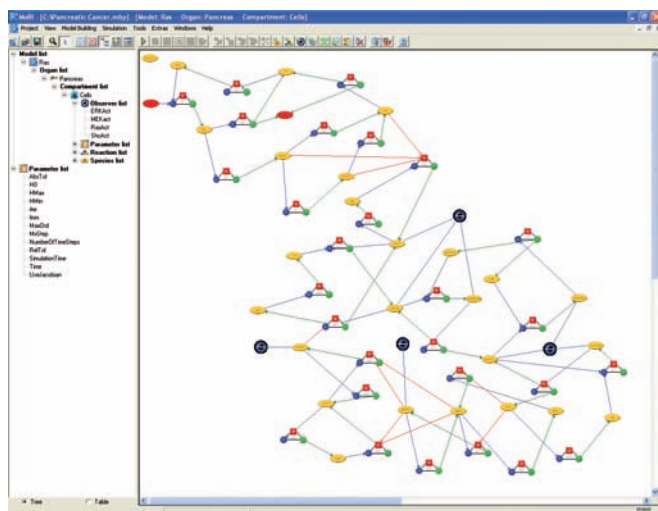




Defining optimization settings

Typical modeling examples illustrating the capabilities of MoBi® are:

- Protein-protein and protein-small molecule interaction networks describing disease mechanisms and pharmacological effects at a sub-cellular level (e.g. signal transduction in the MAPK pathway)
- Auto- and paracrine signaling at a cellular level including cytokine mechanisms and cellular responses like proliferation and apoptosis (e.g. inter-cellular dynamics of a population of B- and T-cells of the immune system in response to an allergic agent)
- Endocrine mechanisms like insulin response to glucose fluctuations embedded in whole-body models at the organism level
- Interactions of a parent compound and its metabolites (no restriction with respect to the number of metabolites) with a full blown mechanistic representation of both the processes of metabolization and the whole-body pharmacokinetics of all compounds
- Dynamic drug-drug interactions including reversible and irreversible enzyme and transporter inhibitions and inductions



Modeling on a molecular level

As a core member of our Computational Systems Biology Software Suite, MoBi® is designed to support your drug research and development program by aiding you to fully exploit the diverse information sources available throughout. By efficient integration of expert knowledge, in-house experimentation and literature based results or models, MoBi® is the tool for model-based knowledge management. It will aid in drawing accurate, invaluable conclusions on which important drug development decisions can be based.

Key Features

- Integrated PK/PD simulations allowing both whole-body physiology and molecular mechanisms
- PK and PD modeling and simulation with an intuitive graphical user interface
- Import of PBPK models generated with PK-Sim® (PK-Sim® PBPK models)
- Execution of simulations and investigation of simulation results by means of a powerful visualization tool
- Combination of multiple PK-Sim® PBPK models
- Integration of PK-Sim® PBPK models with drug action models
- Import/Export to other modeling languages
- Interfaces to MATLAB® and R
- Model optimization and sensitivity analysis within MATLAB®

System Requirements

- OS: Windows XP® or Windows 2000®
- Processor: Pentium III, 500 MHz (1 GHz recommended)
- Memory: 256 MB RAM (512 MB recommended)
- Disk Space: 40 MB (120 MB recommended)

Integrated Solutions and Services

Products	<ul style="list-style-type: none"> • PK-Sim® • MoBi® • MoBi® Toolboxes for MATLAB® and R
Services	<p>Drug Discovery Support</p> <ul style="list-style-type: none"> • Target Identification & Validation • Biomarker Analysis • Proof-of-Mechanism <p>Drug Development Support</p> <ul style="list-style-type: none"> • Species Extrapolation • Extrapolation to Special Populations • Proof-of-Concept • Bioequivalence Studies

For further information on our software tools and services visit our website www.systems-biology.com.

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