

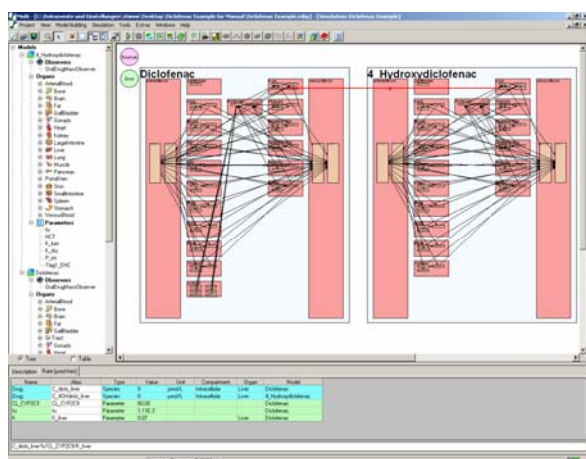
MoBi™

Molecular Biology Modeling and Simulation  
Toolbox

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 attract 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.

**Our Product**

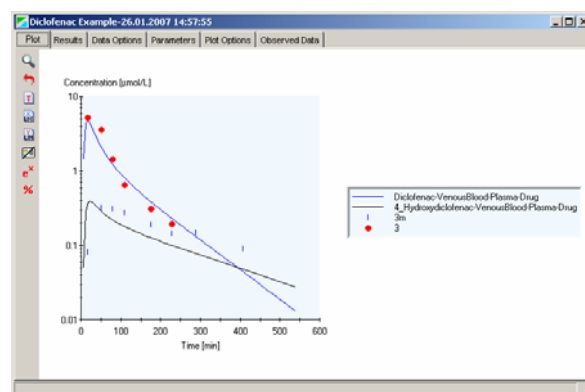
MoBi™ is a sophisticated, flexible software package for mechanistic modeling of biological processes and drug actions. It is completely integrated with PK-Sim® [our package for physiology-based pharmacokinetics (PBPK) modeling] and is, consequently, especially suited for the analysis of complex pharmacokinetic 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.



*Modeling drug-metabolite interaction*

MoBi™ facilitates the process of model building and simulation with its intuitive graphical user interface, the import and export to other modeling languages (e.g.

SBML) and a powerful visualization tool for simulation results. The integration of MoBi™ and Matlab® allows 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 in an automated way.

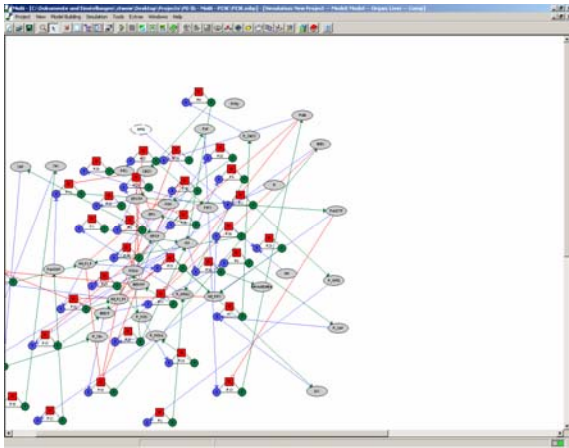


*Comparing experimental data with simulation results*

In the following, a few typical modeling examples are presented that illustrate the capabilities of MoBi

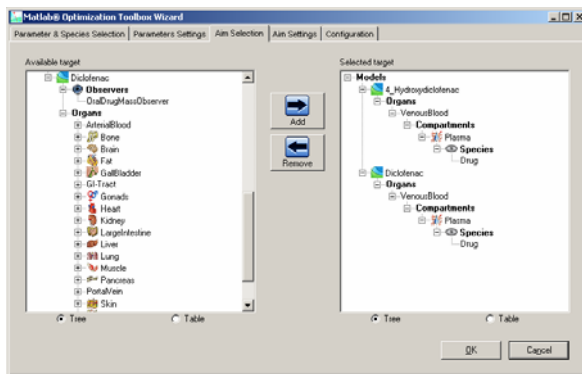
- Protein-protein and protein-small molecule interaction networks describing disease mechanisms and pharmacological effects at a sub-cellular level (e.g. signal transduction in the MAPK pathway)
- Auto- and paracrine signaling at a cellular level including cytokine mechanisms and cellular responses like 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 PK of all compounds
- Dynamic drug-drug interactions including reversible and irreversible enzyme and transporter inhibitions and inductions.





*Modeling on molecular level*

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.



*Defining optimization rules for Matlab*

As a core member of our 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 to base important drug development decisions.

### Key Features

- ✓ Integrated PK/PD simulations comprising 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
- ✓ Interface to Matlab
- ✓ Model optimization and sensitivity analysis within Matlab

### System Requirements

- OS: Windows XP, Windows 2000
- Processor: Pentium III, 500 MHz or better
- Memory: 256 MB RAM
- Disk Space: 40 MB

### Integrated Solutions and Services

BTS offers an integrated suite of products including:

- PK-Sim
- MoBi
- OPAL
- Optimization toolbox

These tools build the platform for our services in the field of mechanistic modelling and simulation:

- ADME Simulation
- Biological Network Modelling
- Evaluation of Drug and Licensing Candidates
- Drug Response Prediction

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