

Drug Response Prediction



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The systems biology group at Bayer Technology Services (BTS) focuses on drug response prediction based on physiological pharmacokinetic and pharmacodynamic models. Our sophisticated approach is the integration and exploitation of knowledge by using these computational models along the whole drug development process. This enables to direct resources leading to savings in both time and money.

Lead finding

- Investigation of the efficacy and adverse effects of new chemical entities by modeling their interactions with key-players within the relevant biological systems

Our Approach to Preclinical Development

An extensive knowledge gain through model-supported analyses efficiently facilitates both the drug discovery by rational selection of the most promising candidate and also the preparation of the clinical development.

Preclinical research

- Execution of efficacy and toxicity studies on virtual animal models
- Identification and quantification of critical and unusual effects (e.g. variability in metabolism, occurrence of active transport)
- Efficient screening of potential biomarkers
- Gain of vast insight in the drug candidates' pharmacokinetics by mapping all relevant processes in a physiologically-based pharmacokinetic (PBPK) model that is validated by in-vitro and in-vivo data

Our Approach to Clinical Development

The developed animal models allow us to extrapolate the preclinical findings to virtual human pharmacokinetics (PK) and pharmacodynamics (PD). Our models are perfectly suited to describe various scenarios that may occur during clinical trials. Especially, they enable us to set up virtual clinical trials of all phases and to actively search for possible complications that may arise in one of the clinical phases. Furthermore, by simulating a population of virtual human subjects, one can anticipate the variability in drug response, identify subpopulations and adjust the clinical trials accordingly. That is why combined PK/PD models are valuable tools to accompany each phase of the clinical development.

Clinical Development

Phase I

- Prediction of the initial dose in humans
- Assessment of safety
- Prediction of drug-drug interactions

Phase II

- Determination of the optimal dose, application form and dosing schedule
- Selection of subjects according to the variability analyses in trial population
- Selection of particular studies by pre-evaluation of their priority

Phase III

- Identification of reasons for unexpected events by in silico hypotheses testing

Phase IV

- Benchmarking of competitor drugs

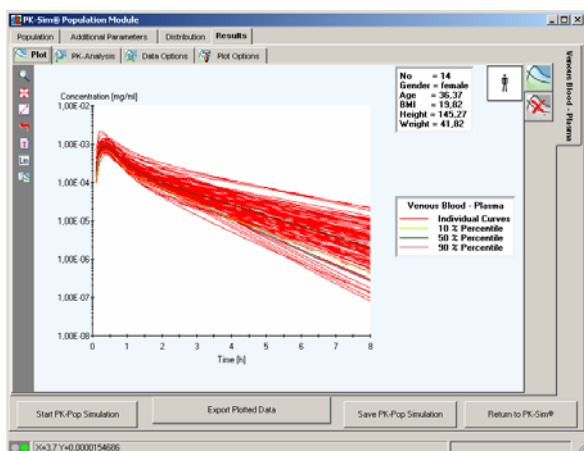




Our Tools and Services

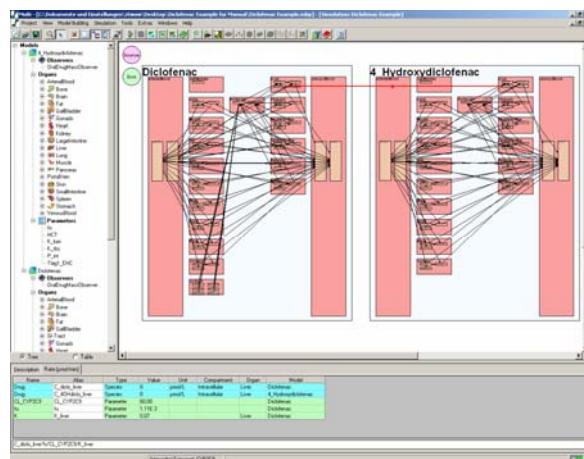
We support our customers by developing and providing mechanistic PK and PD models and applying them along the drug development process. In particular we offer:

- **PK-Sim®** to simulate absorption, distribution, metabolism and elimination of drugs based on whole-body PBPK models
- **MoBi®** for pharmacodynamic modeling of biochemical processes and drug actions on a molecular level
- **Combinations** of PK-Sim® and MoBi® for simultaneous simulations of PK/PD models
- **Consulting Service** based on well-established and appreciated expert know-how



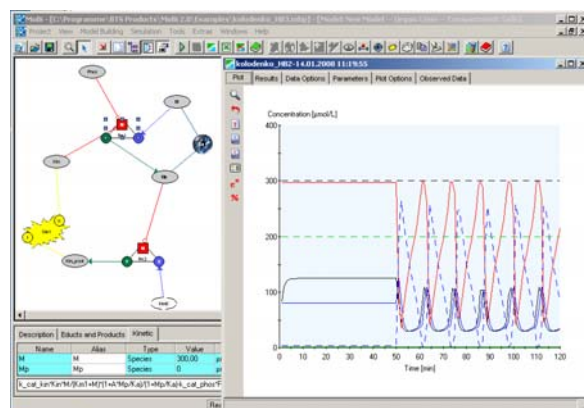
PK-Sim Population Module

Both PK-Sim® and MoBi™ enable to incorporate experimental data conveniently. Therefore, validations, improvements and extensions of the models are straight forward, reflecting the knowledge gain during the clinical trials. Our comfortable software environment is user-friendly and thus, allows easy access to the underlying mechanisms.



Modeling drug-metabolite interaction in MoBi

Shortly, our service includes the interpretation of experimental data, support in the identification and validation of potential drug targets, hypotheses testing, species interpolation and population studies. We help to maximize the knowledge gain from your miscellaneous experimental information. Irrespective of the stage of your R&D project, our cutting edge approach will significantly increase your efficiency. Our in silico studies may compensate for clinical trials partially and hence, save your expenses.



MoBi - modeling on sub-cellular level

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Integrated Solutions and Services

BTS offers an integrated suite of products including:

- PK-Sim
- MoBi

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

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