



Virtual drug trials

To simulate the behaviour of an active ingredient in a living organism, pharmaceutical companies are increasingly working with virtual drug testing. This is made possible by the use of computer-based predictive models, which raise drug research to a new level.

But how does the simulation work and what is needed for it?

With the help of simulation software, it is possible to take into account and simulate all processes from the uptake of an active substance in the body to its distribution and metabolism to its excretion. The simulation enables a data-based prognosis that indicates which path the substance takes in the organism after it has been administered. In addition, it provides important insights into how quickly and through which organ the substance is broken down, as well as information about the effect of the concentration.

The technology determines these predictions on the basis of a database in which a large number of specific key figures of several 10,000 substances are stored. These are analysed for properties such as solubility, molecular weight or protein binding. For further specification, the simulation can distinguish between four species - mouse, rat, dog and human - so that concrete statements about the respective organism can also be made and predicted here.

However, the simulation does not yet provide all the information required for an accurate statement regarding the virtual drug test, which is why an additional evaluation of the coagulation simulator, which can virtually map blood coagulation, is needed. This is a pharmacodynamic computer model that virtually maps the influence of pharmaceutical agents on blood coagulation. The coagulation process simulates how the body stops bleeding when injured - from clotting factors to wound closure and interaction with other proteins. Based on this virtual process, the effect of drugs can thus be examined and tested. At the same time, researchers can change and adjust the parameters to elicit the desired reactions and have them simulated by the prognosis.

INNOVATIVE TECHNOLOGICAL APPROACHES

- ◇ **Company:**
Bayer AG
- ◇ **Technological basis:**
Simulation software
PK-Sim & Coagulation
simulator
- ◇ **Field of application:**
Research & Development
of Medicinal Products
- ◇ **Advantages:**
Simulation and prediction
of the effect of active
pharmaceutical ingredients
in the human organism

Reduction of animal
testing

More efficient drug
development

More targeted and safer
clinical trial planning
- ◇ **Website:**
<https://www.bayer.com/>

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