

In silico Modelling of Skin Absorption – a further Step towards Realizing 3R

Hansen, S.¹, Nägel, A.², Hahn, T.¹, Lehr, C.M.¹, Wittum, G.², Neumann, D.³, Heisig, M.², Schäfer, U.¹

¹Saarland University, Department of Biopharmaceutics and Pharmaceutical Technology, Saarbrücken, Germany

²Simulation and Modelling, Goethe-Center for Scientific Computing, Goethe-University, Frankfurt am Main

³Saarland University, Center for Bioinformatics, Saarbrücken, Germany

To assess potential risks for human health and environment, animal experiments have been a valuable resource. With the REACH legislation, the number of animal experiments may be expected to rise even further.

We present an alternative in silico method, which allows for assessing skin absorption of arbitrary substances and which may help in reducing the number of animal experiments. For this purpose, we have successfully developed a computational model that solves the diffusion equation for discrete points in space and time. Our model allows for computing steady-state permeability coefficients as well as drug concentration-depth profiles after arbitrary times of incubation. It may not only use arbitrary two-dimensional structures, but also more realistic three-dimensional geometries.

Although our work does not replace animal experiments, it may help to reduce the number of animal experiments considerably.

The authors gratefully acknowledge financial support by the “Zentralstelle zur Erfassung und Bewertung von Ersatz- und Ergänzungsmethoden zum Tierversuch” (ZEBET grant FK-3-1228-177) and by the “Deutsche Forschungsgemeinschaft” (DFG grant BIZ 4/1).