Title of Research:

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Establishment of in silico model to predict skin absorption of chemical compounds with two-layered diffusion model

Principal Investigator:

Hiroaki Todo, PhD (Associate Professor, Faculty of Pharmacy and Pharmaceutical Sciences, Josai University)
1-1 Keyakidai, Sakado, Saitama 350-0295, Japan
(tel)+81-049-271-7367

Collaborators:

Kenji Sugibayashi, PhD (Josai University)
Shoko Itakura, PhD (Josai University)
Kenji Mori, PhD (Josai International University, 1 Gumyo, Tougane-shi, Chiba, 283-8555, Japan)
Takeshi Oshizaka, PhD (Josai International University)
Chihiro Takei (Josai International University)
Tetsuya Watanabe (Ohu University) 31-1 Koriyama-shi, Fukushima, 963-8611, Japan
Masahiro Sugino (Ohu University)
Hiroyuki Teramae, PhD (Josai University)

Summary of Research:

The skin is an exposure site for various chemical substances, and predicting the skin permeation rate of a chemical substance is very important for evaluating the safety of the exposed chemical substances. In general, in vitro skin permeation test with excised skin have been applied to estimate skin permeation rates and skin concentrations based on exposure scenarios. On the other hand, since animal testing of all cosmetic products has been banned internationally, it is necessary to establish animal-free testing methods, including systemic toxicity evaluation. Thus, there has been increasing interest in the development of methods to predict transdermal absorption using in silico models. Skin permeability can be expressed by Fick's diffusion law. Therefore, it will be possible to estimate skin permeability when parameters such as diffusion coefficient in skin and partition coefficient to skin of chemical substances can be predicted. In this study, we developed a method to estimate permeation parameters obtained from human skin based on physicochemical properties of chemical substances. Further developed an in silico skin permeation model based on scenarios of dermal exposure to chemical substances and cosmetic formulations. In addition, a software was developed that can easily predict skin permeation by simply entering the structure of the chemical substance with SMILS, the area of application, the concentration applied, and the thickness of the skin. As a result, constructed model was able to accurately predict the amount of chemical substances permeated through the skin with simple web browser-based software.

Timeline:

March 1, 2023- February 29, 2024

Topics:

LRI Annual Workshop（August 25, 2023）
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Publications: