

〈シンポジウム〉

『化粧品の更なる安心・信頼を追求するための新しい視点』

化粧品の安全性評価における *in silico* の活用

上月 裕一

In Silico Methodology for Cosmetic Safety Assessment

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Abstract

In the European Union (EU), the marketing ban of cosmetics tested on animals has been in effect since March 2013 by the 7th amendment of the EU cosmetics directive. On the other hand, The European Centre for the Validation of Alternative Methods (ECVAM) in the EU, the Interagency Coordinating Committee on the Validation of Alternative Methods (ICCVAM) in the United States and the Japanese Centre for the Validation of Alternative Methods (JaCVAM) in Japan have made positive approaches to acquire adoption of alternatives to animal tests as the OECD test guidelines (TG). As the results of their efforts, primary skin irritation test (OECD TG 439), eye irritation test (OECD TG 437, 438), phototoxicity test (OECD TG 432), percutaneous absorption test (OECD TG 428) and genotoxicity test (OECD TG 471, 473) have reached into the OECD TG as alternatives to animal tests. However, alternative methods for skin sensitization test, photosensitization test and some systemic toxicity tests still have not been established since the EU Cosmetic Directive was enforced, because of their intricate toxicity mechanisms. While thinking of such a situation, we have been developing an *in silico* prediction system that might be possible to assess safety risk for cosmetic ingredients by combination of a molecular orbital calculation method and an artificial neural network system, each of which is respectively expected to reflect structural information in detail using descriptors and as a method to clarify the intricate toxicity mechanisms in the body. In addition, we have attempted the prediction for the risk assessment of cosmetic ingredients by the read-across method and category approach using the safety information that was obtained from similar materials considering toxicity mechanism of compounds. In this report, I introduce the approach for safety assessment by *in silico* methods.

Key words: *in silico*, QSAR, read-across, skin sensitization.