日本香粧品学会誌　Vol. 47, No. 1, pp. 1–5（2023）

〈Regular Article〉

Skin Sensitization Potency Prediction of Ingredients in Hair Colorants Using *in silico* Models of Machine Learning

Takao ASHIKAGA[1,*], Kazuto NARITA[2], Mutsumi KOBAYASHI[2], Shigehiro TACHIBANA[2], Wataru MURASAKI[3], Masaharu SUZUKI[3], Kaori AMBE[3], Masahiro TOHKIN[3]

(Accepted: December 11, 2022)

Abstract

Skin sensitization caused by cosmetics, including quasi-drugs, is an extremely serious problem and can become a health hazard. Although several *in vitro* methods for skin sensitization have been established by the Organization for Economic Co-operation and Development (OECD), no practical method for predicting skin sensitization potency has been found which can serve as an alternative to animal testing. In this study, an *in silico* model is developed which predicts skin sensitization potency by combining *in vitro* OECD test guidelines and information of the physical properties of chemicals to evaluate hair dye ingredients without animal testing. A dataset published by Cosmetics Europe was used to develop the *in silico* model. The EC3 value of the mouse local lymph node assay (LLNA), which is used as an indicator of skin sensitization potency, was the objective variable; *in vitro* test values, physical properties, and chemical information obtained from the molecular descriptor calculation software MOE constituted the explanatory variables. CatBoost was adopted as the machine-learning approach. Bandrowski's base (BB), a trimer of the typical oxidative dye para-phenylenediamine (pPD), was used as the test material. In the predictive model, the mean-predicted EC3 value for BB was 0.33%, which meant a strong sensitizer. Furthermore, it was lower than the mean model prediction EC3 value (0.66%) of pPD, which is considered weaker sensitization potency than BB in LLNA. This indicates that BB was correctly predicted as a stronger skin sensitizer than pPD in the proposed *in silico* model.

Key words: skin sensitization, potency prediction, alternatives, machine learning, hair dye.