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〈Regular Article〉

Next Generation Risk Assessment Case Study: A Skin Sensitization Quantitative Risk Assessment for Bandrowski's Base Existing in Hair Color Formulations

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Abstract

Bandrowski's base (BB) is produced from p-phenylenediamine (pPD) in hair dye products during application and is known to have extreme skin-sensitizing potency. We aimed to conduct a quantitative skin sensitization risk assessment using both the predicted EC3 value and the percutaneous absorption rate of BB generated from a machine learning model. We purchased 22 domestically available hair dye products containing pPD and measured the amount of BB produced under simulated product usage conditions. The consumer exposure level (CEL) to BB was estimated using the following parameters: amount of hair dye product applied (100 mL), measured concentration of BB, retention factor (10%), estimated dermal percutaneous rate of BB, and scalp surface area (551 cm^2). The acceptable exposure level (AEL) of BB was determined by converting the local lymph node assay (LLNA) EC3 value of BB to the no expected sensitization induction level (NESIL) value and using a sensitization assessment factor (SAF) of 30, which is commonly set for hair color products. We then used the predicted value of our independently developed machine learning prediction model. Finally, the AEL value was divided by the CEL value for each product to calculate the margin of safety (MOS). The amount of BB generated differed for each product and ranged widely, from below the limit of detection to 38.1 ppm. We calculated the MOS for each product, which was 1 or higher for all products and conditions, similar to the actual measured values of the LLNA EC3. These findings suggest that the use of hair dye products that could generate BB under the evaluated exposure scenarios would unlikely induce skin sensitization. For the practical use of next generation risk assessment for skin sensitization, in addition to comparisons with conventional methods using animals, further verification is necessary, including examination of the validity of tentative set values, test methods, and case studies with other skin sensitizers.

Key words: skin sensitization, Bandrowski's base, next generation risk assessment, machine learning.