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Exposure modeling of chemicals in personal care products

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Abstract: It has been estimated that there are thousands of chemicals used in personal care products (PCPs). To estimate the risks associated with these chemicals, an understanding of toxicity needs to be combined with exposure. Exposure measurements are limited to biomonitoring data, which is only available for a subset of compounds. Models can be used to estimate exposure to chemicals due to the use of PCPs based on physicochemical properties, product composition, and product usage characteristics. The product intake fraction (PiF) can be used to quantify the amount of chemical taken in per mass of chemical used in a consumer product. The PiF can be combined with product composition to estimate exposure to chemicals due to PCP use. We estimated the PiF for hundreds of PCP chemicals and combined several of them with minimum bioactive oral equivalency doses (OEDs) derived from ToxCast AC50s to back-calculate bioactive product concentrations. To understand which physicochemical properties drive use-phase exposure, we calculated PiFs for a range of properties. PiFs were 0.4-100% and 0.001-100% for leave-on and wash-off products, respectively, indicating a variability of about 5 orders of magnitude across PCP chemicals. Calculating the PiF for dermal aqueuous uptake for varying properties indicates that it dominates overall exposure when there is a relatively large Kow compared to a relatively small Kaw such that the chemical does not evaporate from the skin readily. To minimize consumer exposure to PCPs the physicochemical properties would need to be optimized for minimal dermal and inhalation exposure. We compared back-calculated concentrations to values listed in the EPA's Consumer Product Chemical Profile Database which provides product concentration ranges and found that several of the chemicals had back-calculated concentrations less than the mean fractions found in products, indicating that some consumers may be exposed to PCP chemicals at bioactive levels.

Keywords: C-consumer/personal care products, A-exposure models, A-risk assessment, A-chemical prioritization

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Human Urinary Biomarkers of the UV Filter Octocrylene

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Abstract: Octocrylene (OC) is a UV filter substance used in the majority of sun screen formulations and in other personal care products in concentrations up to 10% (maximum authorized concentration within the USA and the EC [1])[2]. OC has been reported to cause photocontact allergy and is of concern owing to possible formation of reactive oxygen species (ROS) in vivo [1,3]. Because of the likely exposure of the general population, OC was selected as a substance of interest by the cooperation project between the German Federal Ministry for Environment (BMUB) and the German Chemical Industry Association (VCI), which has the aim to provide biomarker based exposure data for fifty emerging substances of concern. We investigated metabolism and renal excretion of OC after oral dosage (5 mg) and separately after dermal application. Consecutive urine samples were collected for a period of 48 h or 96 h after dosage, respectively. We obtained crylene acid (breakdown product of OC) and alkyl chain oxidized metabolites as analytical standard substances and analyzed urine samples with online-SPE-LC-MS/MS after enzymatic deconjugation. We could clearly identify the postulated metabolites in post dose urine samples. Elimination characteristics (kinetics), and specificity seem appropriate to use these postulated metabolites as biomarkers of OC exposure for future human biomonitoring studies both in the environmental and occupational field. The study has been approved by the ethical review board of the Ruhr-University Bochum (Reg. No.: 4288-12). References [1] Gilbert et al. International journal of cosmetic science 2013;35:208-19. [2] Kerr et al. Clinical and experimental dermatology 2011;36:541-3. [3] Manová et al. The British journal of dermatology 2014;171:1368-74.

Keywords: A-biomonitoring, A-analytical methods, A-biomarkers