High-throughput exposure modeling to support prioritization of chemicals in personal care products - DTU Orbit (09/09/2017)

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We demonstrate the application of a high-throughput modeling framework to estimate exposure to chemicals used in personal care products (PCPs). As a basis for estimating exposure, we use the product intake fraction (PiF), defined as the mass of chemical taken by an individual or population per mass of a given chemical used in a product. We calculated use- and disposal- stage PiFs for 518 chemicals for five PCP archetypes. Across all product archetypes the use- and disposal- stage PiFs ranged from 10−5 to 1 and 0 to 10−3, respectively. There is a distinction between the use-stage PiF for leave-on and wash-off products which had median PiFs of 0.5 and 0.02 across the 518 chemicals, respectively. The PiF is a function of product characteristics and physico-chemical properties and is maximized when skin permeability is high and volatility is low such that there is no competition between skin and air losses from the applied product. PCP chemical contents (i.e. concentrations) were available for 325 chemicals and were combined with PCP usage characteristics and PiF yielding intakes summed across a demonstrative set of products ranging from 10−8–30 mg/kg/d, with a median of 0.1 mg/kg/d. The highest intakes were associated with body lotion. Bioactive doses derived from high-throughput in vitro toxicity data were combined with the estimated PiFs to demonstrate an approach to estimate bioactive equivalent chemical content and to screen chemicals for risk.

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