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Exposure and Toxicity Modeling of Chemicals in Personal Care Products: Case Study Using Parabens

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Abstract: Chemical prioritization has historically focused on indirect human exposure to chemicals, for example, through the environment, rather than on direct exposure during product use. Furthermore, exposure levels should be combined with toxicity data to more fully understand the risks of chemicals associated with consumer products. Hence, in order to prioritize substances used in consumer products, the entire continuum of usage and emissions, direct and environmental exposure, and toxic effects need to be taken into account. We present a case study on parabens which are used as preservatives in personal care products. We applied the concept of the product intake fraction, PiF (defined as the fraction of chemical taken by the population during product use and disposal) to calculate the exposure to parabens of the U.S. female population via cosmetic products such as shampoo, body lotion, and body wash. The PiF was found to vary between ~1-100% depending on product usage (for example, rinse-off versus leave-on). Exposure during product use was several orders of magnitude higher than exposure through the environment via disposal. Additionally, there can be considerable population variability in exposure factors, such as amount of product used, and uncertainty in factors such as chemical properties. Thus, we used Monte Carlo simulations to take into account population variability and uncertainty. The resulting modeled exposure distributions were within an order of magnitude of urine levels measured in the U.S. female population (NHANES). Furthermore, we used molecular docking models to identify target proteins with which parabens are likely to interact, with particular emphasis on proteins that regulate the endocrine system. Docking studies can be used in conjunction with high throughput toxicity datasets, such as ToxCast from the U.S. EPA, to further inform chemical toxicity. This toxicity information can then combined with the exposure model to identify priority chemicals.

Keywords: A-exposure models, A-chemical prioritization, C-personal care products, C-consumer products, A-aggregate exposure

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Prenatal Exposure to Triclocarban and Triclosan In Relation to Birth Weight and Size in an Urban Population from Brooklyn, NY

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Abstract: Triclosan (TCS) and triclocarban (TCC) are antimicrobial agents formulated in a wide variety of consumer products that are regulated by the U.S. Food and Drug Administration. According to available National Health and Nutrition Examination Survey (NHANES) data, exposure to TCS is prevalent in the general U.S. population. TCS has been detected previously in urine, blood, serum, plasma, human breast milk, and amniotic fluid. In 2014, the FDA is reviewing the use and effectiveness of these chemicals given their potential contribution to bacterial resistance to antibiotics, and endocrine disruption. TCS is known to interfere with thyroid hormone metabolism and has also been associated with allergy and weakening muscle contractibility. TCC has been shown to enhance androgen action and to elicit anti-inflammatory effects. Little is known about potential human effects of either compound in utero. In this study, we assessed prenatal exposure to TCS and TCC and associated birth outcomes including gestational age, birth weight and birth size. We determined the concentrations of TCS, TCC and metabolites as total concentrations in urine and cord blood plasma from a cohort of 181 expecting mothers in an urban, multiethnic population recruited between 2007-'09 in Brooklyn, NY. Maternal characteristics and birth outcomes were gathered from a technician-administered questionnaire and patient charts. We examined the relationship between concentrations of TCS, TCC and metabolites in maternal urine and cord blood plasma with gestational age, birth weight, and birth size. Correlations with birth outcomes yielded insights into the associations with exposure to TCS and TCC. This study is the first to report human biomonitoring data for TCC exposure in an urban population in the United States, and provides additional data on environmental exposure to TCS in the maternal-fetal unit.

Keywords: A-biomonitoring, D-prenatal, C-personal care products, C-consumer products, A-epidemiology