Curating chemical use and exposure predictions to contextualize chemical hazard

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To translate chemical hazard predictions into risk, it is essential to understand how populations interact with and are exposed to various chemical sources. High-throughput in silico exposure simulations and chemical use models can inform exposure scenarios for data-poor chemicals, but the large data volumes associated with these tasks can be challenging for those unfamiliar with computational methods. To provide easily interpretable and accessible exposure and use data, we integrated exposure predictions from EPA's SEEM3 models and use categories from EPA's Chemical and Product Database (CPDat) into the Integrated Chemical Environment v4.0 (ICE; https://ice.ntp.niehs.nih.gov/). Population-level estimates for the 5th, 50th, and 95th percentiles of exposure were obtained from SEEM3, and pathway-specific outputs were used to generate near- and far-field annotations. Predictions were restricted to chemicals within the SEEM3 models' applicability domain. Chemical categories in the ICE Chemical Characterization tool were expanded to include updated consumer use data and functional use from CPDat. Reported functional use terms for nearly 9,500 chemicals were harmonized to OECD functional use categories based on suggested synonyms and expert opinion. To characterize potential use for over 100,000 chemicals that lacked reported functional use, we also added predicted functional use from CPDat to ICE. These predicted uses were curated using a high-probability cutoff to ensure high confidence in results. When presented alongside other toxicologically relevant data within ICE, the addition of these highly curated data provides users with a more comprehensive context for chemical hazard. Project was funded by NIEHS under Contract No. HHSN273201500010C.