Curating Chemical Use Categories and Exposure Predictions to Inform Chemical Assessment

Victoria Hull*[1], Tripp LaPratt[1], Agnes L. Karmaus[1], Kimberly T. To[1], Aswani Unnikrishnan[1], David G. Allen[1], Nicole C Kleinstreuer[2]

[1]Inotiv, Research Triangle Park, NC, USA; [2]NIH/NIEHS/DTT/NICEATM, Research Triangle Park, NC, USA

*Presenting author

To contextualize chemical risk, it is essential to understand how human populations interact with and are exposed to chemicals from various sources. 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 difficult to navigate. To provide easily interpretable and accessible exposure and use data, we integrated predictions from the U.S. Environmental Protection Agency's (EPA's) SEEM3 exposure prediction models and use categories from EPA's Chemical and Product Database (CPDat) into the Integrated Chemical Environment (ICE; https://ice.ntp.niehs.nih.gov/). Population-level estimates of exposure were obtained from SEEM3 for chemicals within the model's applicability domain. Exposure estimates were annotated as "near-field" or "far-field" based on predicted exposure pathways. Chemical use categories in ICE were expanded to include functional use data from CPDat, which describes the roles chemicals serve within products. Functional use terms for nearly 9,500 chemicals were harmonized to categories established by the Organsation for Economic Co-operation and Development based on suggested synonyms and expert opinion. To characterize potential use for over 100,000 chemicals that lacked reported functional use, we added predicted functional use from CPDat. Presented alongside other toxicologically relevant data, this highly curated data will provide users with added context for evaluating chemicals. Further development of ICE will integrate chemical structure classifications using the Classyfire chemical taxonomy from the Wishart Research Group, allowing examination of associations between chemical structures with different use and exposure scenarios. Project was funded by NIEHS, Contract No. HHSN273201500010C.