High Throughput Exposure Estimation Using NHANES Data

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In the ExpoCast project, high throughput (HT) exposure models enable rapid screening of large numbers of chemicals for exposure potential. Evaluation of these models requires empirical exposure data and due to the paucity of human metabolism/exposure data such evaluations include large uncertainty. Wambaugh et al. (2013; ES&T) used CDC National Health and Nutrition Examination Survey (NHANES) as a data source for urinary biomarkers of human chemical exposure and developed an exposure prediction model that had large uncertainties. To reduce the uncertainties, we developed a one-compartment pharmacokinetic (PK) model for relating both serum and urine biomarkers to probable chemical exposures. The PK model was parameterized with metabolic clearance and volume of distribution data compiled from literature sources. This expanded the chemical space explored beyond the urine evaluation chemicals by incorporating serum and blood biomarker concentrations to include environmentally persistent chemicals such as perfluorinated and polychlorinated biphenyl chemicals. Exposures were inferred probabilistically, using Markov Chain Monte Carlo (MCMC) to estimate the distribution of parent chemical exposures consistent with the biomarker data. By incorporating up to 50 additional metabolites from the NHANES data, we reduced the uncertainty in the parent chemical exposure inferences. The incorporation of a more diverse set of metabolites and corresponding reduction in uncertainty in ExpoCast predictions will play a key role in the confident application of exposure models in prioritization and risk assessment contexts. *This abstract does not necessarily reflect EPA policy.*