A Data Repository and Visualization Toolbox for Metabolic Pathways and PBPK parameter prediction

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NHANES is an extensive, well-structured collection of data about hundreds chemicals products of human metabolism and their concentration in human biomarkers, which includes parent to product mapping where known. Together, these data can be used to test the efficacy of applications testing chemical exposure/hazard predictions. To help utilize the data in NHANES reports, we have generated a suite of data and tools to act as a companion to the NHANES reports. First, we assembled chemical parent to metabolism product (p2p) mappings, and created a web application for visualizing the p2p. Second, we collected information of all NHANES chemicals and products, including IUPAC name, common name, NHANES name, CAS number(s), SMILES strings, molecular weight, pKa predictions, logP, and pharmacokinetic parameters derived from two general methods for calculating pK tissue partitioning coefficients for a one-compartment pK model (volume of distribution, fraction unbound, and clearance; where possible). Finally, we combined these data into an R package incorporates the general pK methods and associated algorithms that calculate the fraction of chemical microspecies at each charge state at a particular pH. The collected data is the only publicly available resource for chemical information from the NHANES data, and is a valuable tool for ADME-based chemical exposure inference. The accompanying visualization tool provides further insight into these data, allowing researchers to come up with unique hypotheses for testing. *This abstract does not necessarily reflect EPA policy.*