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PRESENTATION TYPE: Symposium Abstract (Oral)

TITLE: Predicting Exposure Pathways with Machine Learning

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ABSTRACT BODY:

Abstract: Prioritizing the risk posed to human health from the thousands of chemicals in the environment requires tools that can estimate exposure rates from limited information. High throughput models exist to make predictions of exposure via specific, important pathways such as residential product use, diet, and environmental fate and transport. These models can be parameterized in terms of physico-chemical properties that can be predicted with reasonable accuracy from chemical structure. However, as identified by Shin et al. (2015), there are extremely limited data available for identifying the relevant pathways for chemicals in a high throughput manner. Both expert opinion or conservative assumptions (i.e., all chemicals exposed by all pathways) have been considered but have obvious drawbacks. Here we examine the use of machine learning techniques to use structural features and physico-chemical properties to assess the probability that a chemical might be associated with exposure via different pathways. Estimating the relevant pathways using these techniques allows information (including model predictions and other exposure estimates) to be synthesized on a per pathway basis. For each pathway we evaluated the predictive ability of various sources of exposure information using inferred population exposure rates for only those chemicals relevant to the pathway. We can now synthesize exposure models and other predictions commensurate with the ability of those predictions to explain biomonitoring data. In addition, we can attribute the presence of a chemical to specific exposure pathways, potentially allowing structure-based forensic investigation of chemical exposure, and subsequent remediation. The views expressed here are those of the authors and do not necessarily reflect the views or policies of the U. S. EPA.

Shin, H.-M et al., Risk-based high throughput chemical screening and prioritization using exposure models and in vitro bioactivity assays. ES&T 2015, 49, 6760-6771

KEYWORDS: A-exposure models, A-chemical prioritization, A - population exposure, A-statistical methods, A-aggregate exposure.

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