High Performance Environmental Profiling of House Dust to Support Computational Exposure Science

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Only a relatively small subset of chemicals has been sufficiently characterized for potential risks to public health. The desire to increase the pace of risk assessment has led to the development of robust modeling approaches for screening of exposure potential to complement emergent toxicity screening efforts. Models that integrate chemical properties, consumer product information, and modeled human behavior are now being used to evaluate the exposure potential of large numbers of chemicals. Actual measurements of chemicals in exposure-related media are necessary to evaluate the reliability of these models, but data are readily available for only a small number of chemicals, typically those previously identified as possibly posing a hazard to human health. Non-targeted analysis of environmental samples using high resolution mass spectroscopy allows large numbers of chemicals to be measured. We applied liquid chromatography time-of-flight/mass spectrometry (LC-TOF/MS) methods to rapidly screen dust samples obtained from the American Healthy Homes Survey (AHHS). We observed 100 – 1000 peaks in each sample. Using chemical property information from EPA's Distributed Structure-Searchable Toxicity (DSSTox) database, we were able tentatively to characterize many of these to manufactured chemicals. Comparing these chemicals to EPA's Consumer Product Chemical Profiling database enabled us to link dozens of compounds with consumer products. A preliminary analysis of a subset of samples found that the majority of the identified compounds were associated with "beauty" personal care products. High performance environmental profiling of house dust holds great promise for the evaluation and calibration of high-throughput exposure models; moreover, further development and application of the technique to a wider range of environmental media will facilitate the integration of emerging analytical and computational technologies to assess exposure potential on a scale far more grand than previously attainable.

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