

EPA's Non-Targeted Analysis Research Program: Expanding public data resources in support of exposure science

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Suspect screening (SSA) and non-targeted analysis (NTA) methods using high-resolution mass spectrometry (HRMS) offer new approaches to efficiently generate exposure data for chemicals in a variety of environmental and biological media. These techniques aid characterization of the exposome and provide critical information on thousands of chemicals in commerce for which exposure data are lacking. EPA is advancing such techniques with workflows (feature extraction, formula generation, structure prediction, spectral matching, chemical confirmation), and tools (databases; models for predicting retention time, functional use, media occurrence, and media concentration; and schemes for ranking features and chemicals) to rapidly identify, prioritize, and quantify novel compounds in high-interest environmental and biological samples. EPA is also leading a Non-Targeted Analysis Collaborative Trial (ENTACT) to evaluate a range of SSA and NTA approaches. Four categories of experiments are underway, with analyses focused on: 1) ten standard chemical mixtures from the EPA's ToxCast library; 2) extracts of standardized sample matrices (including house dust, human serum, and environmentally deployed silicone passive samplers); 3) extracts of standardized sample matrices spiked with known chemical mixtures; and 4) approximately 4600 single chemicals from the ToxCast library. More than 20 laboratories worldwide from academia, government, and private (i.e., vendor) organizations are participating. Each laboratory is using their own SSA/NTA methods, and will submit results to EPA for performance evaluation and public release. A project goal is to produce benchmark methods for sample and data analysis, as well as results reporting, and to identify areas of future research. A further outcome of this work will be to identify which analytical methods are more suitable to detecting specific classes of chemicals in environmental media. Current progress on these varied NTA/SSA projects and initial results will be presented. *This abstract does not reflect EPA policy.*