Submission for Fall 2021 ACS AGRO Division Session "Nontarget Analyses and Emerging Contaminants: Implications for Agrochemical Risk Assessment"

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Title: State of Non-Targeted Analysis Science and Future Perspectives for Agrochemicals

While somewhat difficult to define, non-targeted analysis (NTA) using chromatography coupled to high resolution mass spectrometry is a useful analytical technique that has the potential to identify a wide range of chemicals in a sample of interest without a predefined list of analytes. NTA is most frequently a qualitative methodology, focused on the identification of compounds. A significant portion of the NTA workflow is conducted after instrumental data to identify compounds and can include large (i.e., millions) chemical databases, predicted retention time or fragmentation spectra, weight of evidence approaches, quality assurance and control, and statistical analyses. Currently, strides are being made towards predicting concentration from NTA analyses without the use of chemical standards. Because chemical standards are not typically involved in NTA, confidence in identification, accuracy, precision, reproducibility, and bounding chemical space investigated are all critical for use of NTA data in a decision making context, but are somewhat ill defined and difficult to assess and report. This presentation will highlight EPA's Non-Targeted Analysis Collaborative Trial (ENTACT) and its efforts to compare NTA results across multiple laboratories using synthetic chemical mixtures of blinded but known composition to characterize these difficult parameters. Chemical coverage by different ionization techniques show that there is significant complementarity between electron impact, electrospray, and atmospheric pressure chemical ionization. Given the range of physicochemical properties of agrochemicals, other formulation ingredients, and their degradates, a range of techniques will likely be desired for maximum chemical coverage. The Benchmarking and Publications for Non-Targeted Analysis (BP4NTA) working group has laid groundwork to harmonize NTA terms and reporting standards, another critical step on the road to proficiency testing and confidence in NTA methodology and data. The study reporting tool provides a framework to assess the reporting quality of NTA studies that can be used by researchers, reviewers, and editors. Finally, we'll discuss some typical uses of NTA data and what the future holds for this rapidly expanding methodology and applications in the agrochemical field. Abstract does not reflect US EPA policy.