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An Introduction to the Benchmarking and Publications for Non-Targeted Analysis Working Group

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ABSTRACT

Non-targeted analysis (NTA) encompasses a rapidly evolving set of mass spectrometry techniques aimed at characterizing the chemical composition of complex samples, identifying unknown compounds, and/or classifying samples, without prior knowledge regarding the chemical content of the samples. Recent advances in NTA are the result of improved and more accessible instrumentation for data generation and analysis tools for data evaluation and interpretation. As researchers continue to develop NTA approaches in various scientific fields, there is a growing need to identify, disseminate, and adopt community-wide method reporting guidelines. In 2018, NTA researchers formed the Benchmarking and Publications for Non-Targeted Analysis Working Group (BP4NTA) to address this need. Consisting of participants from around the world and representing fields ranging from environmental science and food chemistry to 'omics and toxicology, BP4NTA provides resources addressing a variety of challenges associated with NTA. Thus far, BP4NTA group members have aimed to establish a consensus on NTA-related terms and concepts and to create consistency in reporting practices by providing resources on a public Web site, including consensus definitions, reference content, and lists of available tools. Moving forward, BP4NTA will provide a setting for NTA researchers to continue discussing emerging challenges and contribute to additional harmonization efforts.

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