Establishing a Computational Screening Framework to Identify Environmental Exposures Using Untargeted Gas-Chromatography High-Resolution Mass Spectrometry

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Abstract : The human exposome, which includes chemical exposures over the lifetime and their effects, is now recognized as an important measure for understanding human health; however, the complexity of the data makes the identification of environmental chemicals challenging. The goal of our project was to establish a computational workflow for the improved identification of environmental pollutants containing chlorine or bromine. Using the "pattern. search" function available in the R package NonTarget, we wrote a multifunctional script that searches mass spectral clusters from untargeted gas-chromatography high-resolution mass spectrometry (GC-HRMS) for the presence of spectra consistent with chlorine and bromine-containing organic compounds. The "pattern. search" function was incorporated into a different function that allows the evaluation of clusters containing multiple analyte fragments, has multi-core support, and provides a simplified output identifying listing compounds containing chlorine and/or bromine. The new function was able to process 46,000 spectral clusters in under 8 seconds and identified over 150 potential halogenated spectra. We next applied our function to a deidentified dataset from patients diagnosed with primary biliary cholangitis (PBC), primary sclerosing cholangitis (PSC), and healthy controls. Twenty-two spectra corresponded to potential halogenated compounds in the PSC and PBC dataset, including six significantly different in PBC patients, while four differed in PSC patients. We have developed an improved algorithm for detecting halogenated compounds in GC-HRMS data, providing a strategy for prioritizing exposures in the study of human disease.

Keywords : exposome, metabolome, computational metabolomics, high-resolution mass spectrometry, exposure, pollutants

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