Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.15460

Non-Targeted Screening of Biomass Combustion Organic Aerosol with MZmine2 and MFAssignR

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Biomass combustion organic aerosols are highly complex mixtures that significantly impact human health and the world's climate. Therefore, identification and characterization of them are highly important. Ultrahigh resolution mass spectrometry has provided deep insight into the complexity of organic aerosol, but direct infusion methods without chromatographic separation cannot provide structural or quantitative information. Traditionally, liquid or gas chromatography coupled with mass spectrometry used targeted analyte methods, which limit the analysis of aerosol to preconceived compositions. Non-targeted screening methods (NTS) provide a comprehensive analysis, but the instrument and data analysis methods are challenging due to the extreme complexity of natural samples. Therefore, we implemented a new NTS strategy to data obtained from ultrahigh performance liquid chromatography and Fourier transformation Orbitrap Elite mass spectrometer (LC/FT-MS) by using existing data processing software tools, MZmine2[1] and MFAssignR[2]. Commercial liquid smoke was used as a surrogate for biomass burning aerosol. Our method identified 1098 unique molecular formulas corresponding to 3209 molecular species, including structural isomers with positive electrospray ionization (+ESI) mode and 635 molecular formulas with 1697 molecular species with negative electrospray ionization (−ESI) mode. Of these, 970 molecular formulas were common between direct infusion and LC/FT-MS analysis in +ESI, and 590 molecular formulas were common in −ESI for the same sample. The common formulas accounted for 99% of the total peak area in the LC/FT-MS identified species and more than 95% of the total abundance of the direct infusion FT-MS identified species. A correlation between LC/FT-MS peak area and direct infusion FT-MS peak abundance of the commonly identified species was observed. The results demonstrate a significant advance in obtaining structural and semi quantitative information about the molecular level composition of biomass combustion aerosol.

Reference

[1] MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data, Pluskal, T., Castillo, S., Villar-Briones, A., & Orešič, M. (2010). *BMC Bioinform*, *11*, 395.

[2] MFAssignR: Molecular formula assignment software for ultrahigh resolution mass spectrometry analysis of environmental complex mixtures, Schum, S. K., Brown, L. E., & Mazzoleni, L. R. (2020), *Environ. Res*, *191*,110114.