Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.15267

MFAssignR: Software Tools for Molecular Formula Assignment of Complex Organic Matter

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As highlighted by this conference session, the usage of high and ultrahigh resolution mass spectrometry techniques for the analysis of complex organic matter from the air, water, and soil has become more common in recent years. This means there needs to be a way to analyze and assure the quality of this type of data which often contains thousands of individual peaks, each representing at least one molecular compound. Several methods have been developed over the years and each have their advantages and disadvantages related to the purpose for which they were built. Recently, we developed MFAssignR, an R-based open-source package for the formula assignment and data preparation of high and ultrahigh resolution mass spectrometry data with environmental samples as its primary focus. MFAssignR was designed to be an all-in-one package for the preparation and assignment of UHRMS data and thus contains functions for noise estimation, preliminary isotope filtering, internal mass recalibration, and molecular formula assignment with a wide variety of element options (^{12}C, ^{13}C, ^{1}H, ^{2}H, ^{16}O, ^{14}N, ^{15}N, ^{32}S, ^{34}S, ^{31}P, ^{19}F, ^{35}Cl, ^{37}Cl, ^{79}Br, ^{81}Br, ^{127}I) and adducts (Na+, H+, odd electron). These options make it suitable for use with positive and negative mode electrospray, APCI, and APPI. MFAssignR is also suitable for direct infusion samples and liquid chromatography samples due to its ability to retain retention time information and isomeric molecules (same m/z with different RT). In this presentation, I will describe how the functions work, how they can be used for various types of studies, and highlight a few studies from various research groups that have used MFAssignR for their work in recent years.

[1] Schum, Brown & Mazzoleni (2020), *Environmental Research*, https://doi.org/10.1016/j.envres.2020.110114