Guided analysis of ambient ionization mass spectrometry data with the MQ_Assistant

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Abstract

RATIONALE Ambient ionization mass spectrometry (AIMS) delivers realistic data from samples in their native state. In addition, AIMS methods reduce time and costs for sample preparation and have less environmental impact. However, AIMS data are often complex and require substantial processing before interpretation. METHODS We developed an interactive R script for the guided processing of mass spectrometry (MS) data. The 'MQ_Assistant' is based on MALDIquant, a popular R package for MS data processing. In each step, the user can try and pre-view the effect of chosen parameters before deciding on the values with the best result and proceeding to the next stage. The outcome of the MQ_Assistant is a feature matrix that can be further analyzed in R and statistics tools such as MetaboAnalyst. RESULTS Using 360 AIMS example spectra, we demonstrate the step-by-step processing for creating a feature matrix. In addition, we show how to visualize the results of tree biological replicates of a plant-microbe interaction between Arabidopsis and Trichoderma as a heatmap using R and upload them to MetaboAnalyst. The final parameter set can be saved for reuse in MALDIquant workflows of similar data. CONCLUSIONS The MQ_Assistant helps novices and experienced users to develop workflows for (AI)MS data processing. The interactive procedure supports the quick finding of appropriate settings. These parameters can be exported and reused in future projects. The step-wise operation with visual feedback also suggests the use of the MQ_Assistant in education.

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