

Alternating in-source fragmentation with single-stage high-resolution mass spectrometry with high annotation confidence in non-targeted metabolomics

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Abstract	<p>Non-targeted metabolomics is increasingly applied in various applications for understanding biological processes and finding novel biomarkers in living organisms. However, high-confidence identity confirmation of metabolites in complex biological samples is still a significant bottleneck, especially when using single-stage mass analysers. In the current study, a complete workflow for alternating in-source fragmentation on a time-of-flight mass spectrometry (TOFMS) instrument for non-targeted metabolomics is presented. Hydrophilic interaction liquid chromatography (HILIC) was employed to assess polar metabolites in yeast following ESI parameter optimization using experimental design principles, which revealed the key influence of fragmentor voltage for this application. Datasets from alternating in-source fragmentation high resolution mass spectrometry (HRMS) were evaluated using open-source data processing tools combined with public reference mass spectral databases. The significant influence of the selected fragmentor voltages on the abundance of the primary analyte ion of interest and the extent of in-source fragmentation allowed an optimum selection of qualifier fragments for the different metabolites. The new acquisition and evaluation workflow was implemented for the non-targeted analysis of yeast extract samples whereby more than 130 metabolites were putatively annotated with more than 40% considered to be of high confidence. The presented workflow contains a fully elaborated acquisition and evaluation methodology using alternating in-source fragmentor voltages suitable for peak annotation and metabolite identity confirmation for non-targeted metabolomics applications performed on a single-stage HRMS platform.</p>
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