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Development of bioinformatics tools towards automated structural elucidation of unknowns from MS/MS spectra

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Metabolomics relies on liquid chromatography coupled to mass spectrometry to detect and identify metabolites for two principal reasons: (i) the high throughput capability of LC-MS/MS and (ii) the high sensitivity of LC-MS/MS. While high resolution mass spectrometry allows the determination of elemental formulae for precursors, compound identification is generally based on library searches or the use of fragmentation rules of postulated structures and fragment ions. Here we propose a method for automated substructure assignment to peaks from MS/MS spectra. We have applied hierarchical clustering to m/z values gathered from high-resolution MS/MS data in the Riken dataset. Using constraints of parent compound structure and elemental composition, we propose substructures for fragments in large clusters. We also evaluate the utility of this tool by benchmarking annotations against MS/MS data gathered from the IPB Leibniz dataset. Together with neutral loss clustering, we believe that our tool can be very useful in the annotation of spectra from unknown compounds.

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