Dynamic Cluster Analysis: An Unbiased Method for Identifying A+2 Element Containing Compounds in Liquid Chromatographic High-Resolution TOF Mass Spectrometric Data - DTU Orbit (06/05/2019)

Dynamic Cluster Analysis (DCA) is an automated, unbiased technique which can identify Cl, Br, S, and other A+2 element containing metabolites in liquid chromatographic high resolution mass spectrometric data. DCA is based on three features, primarily the previously unutilised A+1 to A+2 isotope cluster spacing which is a strong classifier in itself, but improved with the addition of the monoisotopic mass, and the well-known A:A+2 intensity ratio. Utilizing only the A+1 to A+2 isotope cluster spacing and the monoisotopic mass it was possible to filter a chromatogram for metabolites which contain Cl, Br, and S. Screening simulated isotope patterns of the Antibase Natural Products Database it was determined that the A+1 to A+2 isotope cluster spacing can be used to correctly classify 97.4% of molecular formulas containing these elements, only misclassifying a few metabolites which were either over 2800 u or metabolites which contained other A+2 elements, such as Cu, Ni, Mg, and Zn. It was determined that with an inter-isotopic mass accuracy of 1 ppm, in a fully automated process, using all three parameters, it is possible to specifically filter a chromatogram for S containing metabolites with monoisotopic masses less than 825 u. Furthermore, it was possible to specifically filter a chromatogram for Cl and Br containing metabolites with monoisotopic masses less than 1613 u. Here DCA is applied on: i) simulated isotope patterns of the Antibase natural products databases; ii) LC-QTOF data of reference standards; and iii) LC-QTOF data of crude extracts of 10 strains of laboratory grown cultures of the microalga Prymnesium parvum where it identified known metabolites of the prymnesin series as well as over 20 previously undescribed prymnesin-like molecular features.

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