

Fayda: A data processing, visualization, and predictive platform for atomic ICP-MS/MS.

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The Fayda application is a data visualization, analysis, and predictive platform developed to facilitate data acquisition and analysis with atomic tandem inductively coupled plasma mass spectrometry (ICP-MS/MS). Fayda's visualization and analysis features automate basic data processing of small to massive data sets, including sorting, labeling, calculating errors, and performing blank subtractions. Selective extraction of data from single runs, or multiple runs over an extended period of time can also be performed, such as for assessing signal stability. Consistent background signals from plasma, reaction gas, and matrix species can be visualized and removed from the data set. Mass spectra across multiple data sets can be plotted individually or on the same plot for easy comparison of isotopes of either the same or different elements. Fayda also has the natural isotopic abundance ratios built in which allows for overlays to be plotted with the data for basic data interpretation. In the near future, Fayda will also contain Density Functional Theory (DFT) derived thermochemistry data and will also be able to calculate ion kinetic energies in the collision cell using previously established models. These additions will allow Fayda to predict the reactivity of an ion with a given reaction gas and would be able to recommend the type of reaction gas and the tuning parameters that would be optimal for separating analyte/interference pairs.