Constructing a mass accuracy surface can improve automatic annotations in LC-MS based Metabolomics

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Metabolite annotation is one of the major challenges in mass spectrometry (MS) based untargeted metabolomics, and is essentially depending on exact mass measurements. The quality and efficiency of annotations can be strongly improved by the development of innovative strategies, including ones for a precise evaluation of mass accuracy in the data analysis pipeline. The quadrupole time of flight mass spectrometer (Q-TOF-MS), often used for metabolomics studies was evaluated several times in the past in order to find the important factors affecting mass measurements in terms of accuracy and precision, but the applicability of these studies for large scale untargeted essays is largely limited. In this presentation, I will demonstrate that the quality of peak annotations can be improved by using an adaptive mass accuracy window, estimated by a continuous surface function which is constructed by analyzing an extensive data set of authentic chemical standards. A practical application of the model will be presented.