Integrating mass spectrometry (MS)-based metabolomics, the untargeted detection and relative quantification of literally all metabolites in a biological system has become a powerful discovery tool in many scientific disciplines. With respect to MS methodology, for making sense of the resulting data we need to process the raw data to detect unique chemical species, assign particular to specific metabolites, and integration of these raw data into a coherent and globally meaningful processed multi-omics framework that can yield a full understanding of the biological system (Figure 1A). For the first step of thisinformatics-driven data processing (Figure 2), critical for the success of the metabolomic study, data processing generally consists of three computational steps: peak detection, peak grouping and alignment for LC-MS and spectral deconvolution for GC-MS. GC-MS alignment. While many existing software tools have been developed specifically considering the complex nature of the data, the underlying algorithm to each step of the data preprocessing may vary extensively. Here we present a new and more comprehensive data processing tool that is not to detect and data to be clustered and analyzed. Alignment algorithms that are not performed well for low abundance peaks of a target molecule yield will definitely affect the results of the study. ADAP-GC 2.0 can be used as a tool for fast automatic spectral deconvolution and alignment for GC-MS and TOF-MS data.

ADAP-GC has been implemented in our research team and has been found to be advantageous for the analysis of GC-MS and TOF-MS based metabolomics studies.