Mass-suite - Novel data analysis package for mass spectrometry data for water quality assessment

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Mass-suite is a python based open source package that designed to utilize High Resolution Mass Spectrometry (HRMS) data for water quality assessment. The analysis of HRMS data for water quality assessment is still in its infancy, with many basic aspects of data reduction, analysis, and interpretation still lightly developed. Here, the package is providing flexible and various capacity to process the HRMS data from basic functions to advance data analysis, such as dilution rate prediction and source tracking analysis, and will fill the gap left by current software. The package is developed in a modularized concept so that the user can use different combinations of parts of our code to accomplish their tasks. By providing this package, we hope to open up a new space for HRMS data analysis, resulting in more rapid and detailed research in the area.