Quantification and Isomer Differentiation of PFAS at ppb/ppt Levels using MALDI-TOF with Trapped Ion Mobility

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Poly- and perfluoroalkyl substances (PFAS) are a class of organic compounds that have attracted global attention for their persistence in the environment and adverse health effects in biological systems. There is an urgent need to develop analytical methodologies for quantification and characterization of PFAS in various sample matrices. Current efforts in PFAS characterization research have centered around chromatography-coupled tandem mass spectrometry. While chromatography-based methods have many advantages, they require extensive sample preparation, require longer analysis times, and are prone to contamination. Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) is a chromatography-free mass spectrometry method that performs laser-based ionization and *in situ* analysis on samples. Herein we present the results for PFAS detection and quantification by MALDI-TOF-MS with trapped ion mobility (TIMS) for detection, quantification, and isomer differentiation of perfluorocarboxylic acids (PFCAs) and perfluorosulfonic acids (PFSAs). MALDI matrix composition and key instrument parameters were optimized to produce different ranges of calibration curves. We achieved quantification and detection of PFCAs at parts per billion (ppb) concentrations and PFSAs at parts per trillion (ppt) concentrations. The repeatability of calibration curves was examined by multi-day calibration curves and assessed by calculating linear dynamic ranges, limit of detection, and limit of quantification. Using TIMS, we also successfully separated three perfluorooctanesulfonic acid structure isomers in the gas phase. Our results demonstrated the new development of utilizing MALDI-TOF-MS coupled with TIMS for fast, quantitative and sensitive analysis of PFAS, paving ways to future high-throughput and *in situ* analysis of PFAS such as MS imaging applications.