

An increasing number of studies have been conducted to investigate the environmental distribution of perfluorinated alkyl compounds (PFCs), many of which are known to be toxic in laboratory animals. Despite growing public concerns, fate and transport of PFCs are little known. Many studies have presented wastewater treatment plants (WWTPs) to be possible major contributors to the surface water environment. In order to investigate the impact of WWTPs on PFC load to the surface water environment, precursor compounds that potentially degrade to PFCs in WWTP process should be identified and quantified together with PFCs. Existing metabolite structural analysis software coupled with the Ion-Trap Time-of-Flight (IT-TOF) mass spectrometer was modified and applied to extracts of WWTP samples. Samples were run on a high-performance liquid chromatography equipped with IT-TOF. MSⁿ spectra were obtained automatically by programming the instrument to acquire the MSⁿ scan when each chromatographic peak hit a threshold. Each precursor was identified using accurate mass (< 5 ppm), MSⁿ spectra, isotope pattern matching, carbon-hydrogen ratio, and nitrogen rule. Utilizing the software spectra for precursor materials were extracted from large data sets and associated with the terminal PFC species. The details of the technique and identified precursors will be presented.