Development of an Organofluoride Method to Quantify Total Per- and Polyfluoroalkylated Substances (PFAS)

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Background/Objectives. Per- and polyfluoroalkyl substances (PFAS) are a huge class of chemicals that are widely used for many commercial and industrial applications. There are more than 3000 PFAS reported to be in the market to date. Out of these, the known quantifiable PFAS account for a very small fraction and only a limited number of analytes can be quantified using the targeted analysis. Hence, there is a need for a method that can be used to quantify the total fluorine present in environmental samples. The current study investigates a proof of concept approach to break down the total PFAS into free fluoride and quantify the fluoride generated using ion selective electrode and ion chromatography techniques.

Approach/Activities. A rapid screening method was developed to measure the free fluoride generated by the quick reductive defluorination of PFAS in environmental samples. Different quantitative methods were tested to quantify the free fluoride formed. Fluoride quantification was performed using an ion selective electrode, ion chromatography techniques, and a quantitative 19F NMR technique for accurate quantification and confirmation of free fluoride concentrations. In addition, non-targeted analysis was also performed to understand the mechanistic details of the fluoride generation from the parent compound using different conditions. This technique was tested on both the shorter and longer chain perfluorinated carboxylic acids, sulfonates and precursor chemicals.

Results/Lessons Learned. The results show that this novel total organofluoride method can be used as a rapid screening tool to measure the free fluoride generated in environmental samples. Consistent results were obtained from different fluoride quantitation methods. This method can be used as a quick tool to identify the total fluoride present in the samples without using time-consuming instrumentation.