

# Optimizing Perfluorooctanoic Acid (PFOA) Detection in Surface Water Samples through Derivatization in Gas Chromatography Mass Spectrometry

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Per- and polyfluoroalkyl substances (PFAS) encompass a broad array of organic molecules featuring fully or partially fluorinated hydrophobic carbon chains linked to various hydrophilic functional groups. PFAS find applications in over 200 diverse sectors, varying from industrial-mining practices to food production and firefighting foams. This widespread usage is attributed to the chemical and thermal stability of the carbon-fluorine bond, along with its exceptional capability to repel both oil and water. PFAS exhibit a slow degradation rate in the environment and considered as “forever chemical” of global significance. Detection PFAS in natural systems remains relatively unexplored, with significant gaps in our understanding. Liquid chromatography-mass spectrometry has emerged as a preferred method for determining PFAS since 2001, addressing limitations of gas chromatography mass spectrometry. Currently, PFAS analysis using GC-MS remains underutilized. Nevertheless, it is crucial not to ignore the cost-effectiveness and widespread availability of GC. It can identify PFAS isomers/derivatives in environmental and biological samples due to its high-resolution capabilities. This study presents an optimized method for detecting perfluorooctanoic acid (PFOA) which belongs to the class of PFAS in surface water samples using derivatization in GC-MS, significantly enhancing the efficiency of detection. To increase the efficiency of PFOA detection, we have used N, O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) and trimethylchlorosilane (TMCS) (99:1, v/v). A linearity plot correlating mass spectrometry signal with varied concentration was generated by analyzing PFOA across a dynamic range of 1–500 ng/mL, with three replicates per data point using 8860 GC, 5977B MS (Agilent Technologies®).