

## Ph.D. DISSERTATION DEFENSE

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<b>Degree:</b>	Doctor of Philosophy
<b>School/Department:</b>	Charles V. Schaefer, Jr. School of Engineering and Science / Chemistry and Chemical Biology
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<b>Title:</b>	Investigation of Ultra Performance Liquid Chromatography and Traveling-wave Ion Mobility Procedures in Mass Spectrometry for Analyzing Mixtures
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### ABSTRACT

Mixtures are ubiquitous in chemistry, ranging from simple combinations of two or more substances to complex formulations encountered in various natural and synthetic contexts. Mixture analysis involves the identification and quantification of individual components within a mixture, elucidating their concentrations, interactions, and structural characteristics. Modern instrumental techniques, including chromatography, spectroscopy, and mass spectrometry (MS), have been developed to address the diverse challenges posed by mixture analysis. In this dissertation work, the procedures of ultra-performance liquid chromatography (UPLC) MS and ion mobility (IM) MS used to analyze mixtures were investigated.

During the method development for the quantification of per- and polyfluoroalkyl substances (PFAS) by UPLC-MS, the presence of two chromatographic peaks have been noted under certain experimental conditions from the same analyte: one for the expected retained peak and one for an unexpected peak at a very early elution time (breakthrough peak). The phenomenon of breakthrough in liquid chromatography has been known for decades. In this project, a comprehensive study was carried out to uncover the underlying mechanisms. I discovered that this breakthrough can occur even when a sample of a neat solvent, devoid of any solute, is injected. My results showed conclusively that it is the micelle formation by a nonionic detergent present in aqueous phase as a contaminant that results in this undesired breakthrough in UPLC.

When dealing with mixtures of isomers, in addition to chromatography and MS, IM provides another dimension of differentiation based on the shape of gaseous ions. After optimizing the key parameters, an IM-MS procedure was used to separate phenyl sulfate, a biomarker, from its isomer, phenol sulfonate. Compared with LC-MS, the IM-MS method achieved baseline separation and took only milliseconds for an analytical cycle. In another project, the arrival time distribution profiles obtained by IM-MS was successfully used to differentiate the 3 regioisomers of sulfobenzoic acid.