

## A76 Liquid Chromatography - Tandem Mass Spectrometry Analysis of Organic Compounds in Soil

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After attending this presentation, attendees will gain a better understanding of soil analysis and the ability of a Liquid Chromatography - Tandem Mass Spectrometry instrument (LC-MS/MS) to analyze and differentiate the organic components of soil.

This presentation will impact the forensic science community by demonstrating the development of an objective method that may be used to analyze and discriminate obtained soil evidence.

Soil evidence can be important in forensic science cases as it contains many compounds that can be analyzed, including minerals and organic compounds. Unfortunately, most current analysis methods involve subjective analyses: comparisons of particle size, color, and type. The use of a more objective method, Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS), can eliminate the inherent bias present in those subjective methods and lead towards a more accurate and reliable soil analysis. Soil samples vary more from each other when comparing between two areas separated by a large distance. In this research, however, the sampling area was kept small and limited to the area of Allegheny County, Pennsylvania. Previous research was conducted analyzing the mineral composition of the soils from the same regions. This research focused on an analysis of the organic components of the soil and the variability of the organic composition in a small geographical area.

Soil samples were obtained from locations across Allegheny County. An organic solvent was used to extract the organic compounds from the soil, and the resulting extract was analyzed using LC-MS/MS. The mass spectrometer used was a Triple Quadrupole Mass Spectrometer (QqQ). By using the LC-QqQ instrumentation, tandem mass spectrometry experiments, like multiple reaction monitoring (MRM), could be developed to increase the sensitivity of the analysis.

Early experiments used acetonitrile as the extraction solvent and a 100% water to 100% acetonitrile mobile phase gradient with a C18 column. These results showed poor resolution and difficulty in distinguishing soil extraction samples from extraction solvent blanks. In later experiments, different organic solvents, (e.g. acetone, isopropanol, methanol, and tetrahydrofuran) were used as the extraction solvents. Different mobile phase compositions were also used, including a 100% methanol to 100% acetonitrile and a 100% methanol to 100% acetone mobile phase gradient. A more polar cyano column to improve the separation and analysis of the soil samples was also tested.

Preliminary results have shown an increase in resolution and peak differences between samples using the methanol mobile phase gradients and the cyano column. These methods will continue to be further researched and optimized. An optimized scanning method will be used to set up a precursor ion scan method, which will determine how the soil components are being fragmented. These results will then be used to set up an MRM method. The development of an MRM method for the analysis gives a discrete set of variables that can be used for the characterization of each individual soil sample. The optimized MRM method then allows for a comparison between all collected soil samples for each MRM parameter.

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**Liquid Chromatography, Mass Spectrometry, Soil Analysis**