A92 Utilizing Comprehensive Gas Chromatography Coupled to Fast- Scanning Time-of-Flight Mass Spectrometry for the Analysis of Forensically-Relevant Samples

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After attending this presentation, attendees will gain an understanding of the technique of comprehensive gas chromatography, or GCxGC, and how this technique can aid the forensic chemist for a variety of analyses including fire debris and drug analysis. Additionally, the benefit to the legal system will also be discussed, where the output from this technique may be more easily explainable and understandable to the court.

This presentation will impact the forensic science community by educating potential users of this technique as to its abilities, and how they might be used in a variety of analytical methods to provide greater data quality, and also easier comprehension to a non-scientific audience such as the legal system.

Comprehensive GCxGC is a relatively recent technique available to separations scientists. Largely credited to Phillips, this technique has recently become more user-friendly, robust, and accepted in the scientific literature.[1,2] Additionally, several systems are now available to potential users, which increases the potential for application to the field of forensic science.

This presentation will address the fundamentals and instrumentation for GCxGC. Specifically, the use of cryogenic modulation GCxGC coupled to Time-Of Flight Mass Spectrometry (TOF-MS) will be discussed, allowing for an increase in chromatographic peak capacity and sensitivity for many complex separations. This increase in peak capacity allows for higher data quality when analyzing complex samples. Through the examples of fire debris and drug analysis, this presentation will demonstrate that GCxGC-TOF-MS should be considered as a viable analytical technique in the forensic science field because: (1) it allows for the classification of compounds based upon chemical functionality, thus allowing for tentative peak assignment even in the absence of reference standards; (2) it allows for greater peak resolution which improves both qualitative id and quantification accuracy; (3) it allows for data display that is much more easily explained to members of the legal community who may not have years of analytical chemical education and experience; and, (4) it may allow for identification of marker compounds and other trace compounds that are obscured for a variety of reasons in more conventional analyses.

Specific examples of pharmaceuticals in wastewater samples and data from an arson case will be presented to briefly demonstrate the benefits of this technique. The analysis of drugs in wastewater may allow for spatial and temporal resolution of usage in a population, but the analysis conditions are difficult using conventional approaches. Many of the drug compounds and metabolites are at very low levels of concentration relative to the variety of co-extractable, or matrix, compounds that are also found in wastewater. If these matrix compounds are not resolved in the chromatographic analysis, they may either obscure the trace compounds or bias the mass spectrum such that detection becomes difficult. GCxGC-TOF-MS data will be shown in comparison to GC/MS data to demonstrate the utility of the technique.

Equally, fire debris samples present a difficult separation. Most potential accelerants are hydrocarbon-based distillation fractions, and contain a large number of individual compounds. In some cases (diesel and kerosene, for example), these materials can be difficult to distinguish from one another, especially once they have been weathered either through evaporative loss or through combustion. Again, the increased peak capacity and selectivity of GCxGC-TOF-MS will be compared to the more conventional GC/MS technique to demonstrate the benefits of the use of this technique to the forensic community.

References:

1. Phillips JB, Liu Z. J Chromatogr Sci 1991;29:227-231.
2. Phillips JB, Xu J. J Chromatogr A 1995;703:327-334.

Fire Debris, Drug Analysis, GCxGC/TOF-MS

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