



K59 Discovery-Based Analyses of Wastewater Samples for Characterization of Drug Usage

Adrienne W. Brockman, BS*, 107 Whitmore Labs, University Park, PA 16802; Jack Cochran, BS, 110 Benner Cir, Bellefonte, PA 16823; Michelle Misselwitz, BS, 110 Benner Cir, Bellefonte, PA 16823; and Frank Dorman, PhD, 107 Whitmore Labs, University Park, PA 16802

After attending this presentation, attendees will understand the principles and design of Wastewater Treatment Facilities (WWTFs) and how these locations and wastewater systems in general may be used to determine temporal and spatial trends in the usage of a wide variety of compounds. Monitoring human usage of several categories of controlled substances can yield the information to allow for either targeted enforcement or targeted education. Additionally, the location of possible synthetic operations may be determined through the monitoring of wastewater. This may aid law enforcement in focusing their efforts in a certain region. Additionally, attendees will have a better understanding of appropriate extraction methods used to recover specific analytes from wastewater and also know what steps can be taken to identify and quantify the analytes of interest.

This presentation will impact the forensic science community by providing a mechanism to inform law enforcement and community leaders on community drug habits by the development of a method for monitoring wastewater. Questions such as the following can be answered using this approach: In what areas/neighborhoods are drugs being consumed? What drugs are being consumed? In what volumes are drugs being consumed and in what usage patterns? This could help pinpoint at-risk populations for drug abuse, which may help tailor the drug education curriculum in specified school districts. This could also help facilitate law enforcement in combating areas with identified drug usage.

The information obtained through the monitoring of WWTFs may be used for a variety of purposes. The objective of this research is to determine compounds present in wastewater samples specifically obtained from the Pennsylvania State University wastewater treatment plant, which is being used as a control facility to refine analytical methodology. Rather than beginning with a target compound approach, a discovery analysis approach was chosen to attempt to determine as many compounds as possible prior to any compound list restriction. The difficulty in this approach can be the resulting complexity of the analysis. For this reason, utilization of both Comprehensive Gas Chromatography coupled with Time-Of-Flight/Mass Spectrometry (GC x GC/TOF/MS) analysis and also High Performance Liquid Chromatography coupled with Time-Of-Flight/Mass Spectrometry (HPLC/TOF/MS) analysis were chosen for their inherent ability to characterize these potentially complex samples more successfully compared to other possible techniques. Several categories of compounds were found using this approach in the initial discovery experiments. Specifically, a number of antidepressants (SSRI's and MAOI's), synthetic opioids, and steroids, were found in addition to a number of endocrine disrupting compounds. Additionally, a series of chlorophenyl cyanates were found, which may indicate a chemical synthesis operation, though likely not an illicit drug facility. The determination, through spatially-resolved sampling, of the source will serve as a model for how other synthesis operations could be uncovered and located through the use of this procedure. An example of the complexity of the analysis is revealed through inspection.

Once the discovered compounds are identified and quantified, the ultimate goal is to determine when and where these compounds were introduced into the wastewater system. Employing time-resolved sampling at locations upstream from the WWTF, both the location and the usage patterns were narrowed down. Although a large array of compounds could be identified in the wastewater, this research project will focus particularly on drugs and drug metabolites.

For the discovery phase, samples of wastewater were gathered by "grab" sampling from the Penn State WWTF. Multiple four-liter samples were gathered from each of the following: influent flow, effluent flow, three intermediate stages, and final spray effluent. Following USEPA method 3510, a liquid-liquid extraction process was performed to demonstrate a "baseline" to compare with other extraction methods. A separatory funnel was used for extraction purposes, with methylene chloride as the solvent. Immediately following, the Kuderna-Danish technique was used to concentrate the samples to 1mL. Once the samples had undergone the clean-up process, they were introduced to the analytical systems to identify and quantify the compounds.

The presentation will discuss the methods used to extract, identify, and quantify the analytes of interest. Also, in the discussion, Pharmaceuticals And Personal Care Products (PPCPs) will be brought to the forefront for conversation, as this research project's focus also covers PPCPs as well as emphasizing drugs and drug metabolites.

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