SOAR Research Proposal - Summer 2018

Drug Analysis of Wastewater Using Gas Chromatography-Mass Spectrometry
Faculty: Alison Holliday, Assistant Professor of Chemistry
Student: Madison Pursell'19
Project Start Date: June 4, 2018
Length of Project: 10 weeks

Description of the Project:

The main focus of Madison's research will be to determine the amount of drugs and their metabolites in Bethlehem wastewater. This type of research is a non-invasive approach to determine the extent of drug use in an area. The drugs that are consumed are passed intact or metabolized by the body; the drugs and their metabolites are thus excreted through urine and end up in wastewater. The primary drugs that will be investigated are commonly used illicit drugs, such as heroin, fentanyl, methamphetamine, and cocaine.

This is a continuation and an expansion of research from Madison's spring half unit independent study. During her independent study, she started to develop a method to detect a metabolite of heroin, 6-acetylmorphine, using gas chromatography-mass spectrometry (GC-MS). A method needed to be created because 6-acetylmorphine, as well as every drug mentioned above, is too polar to analyze directly with the GC-MS. A derivatization procedure needs to be developed for all of the above mentioned drugs to make them all non-polar. Due to the different properties of the different drugs, a single procedure and derivatizing reagent will probably not work for all of them. However, Madison will be investigating whether the derivatization can occur in "one pot" (i.e. using multiple derivatization reagents concurrently or consecutively on the same sample).

After a derivatization procedure is optimized, different concentrations of the derivatized drug need to be introduced into the GC-MS so that when testing wastewater, it can be determined how much of the drug is present. The concentration of drugs and their metabolites will (hopefully!) be very small in the wastewater, and so solid phase extraction will be used to extract and concentrate the drugs, and other positively charged things, from surrounding wastewater. As extraction may not capture 100% of the drug molecules present, deuterated standards will be added before extraction to compensate for the loss. Tests will be run to verify that the drug and the deuterated standard are readily distinguished on the GC-MS.

We have contacted the Bethlehem Water Authority and have permission to collect wastewater samples. However, working with untreated wastewater may be an issue as it may be unsafe as a biological sample. Autoclaving would make the sample biologically safe, but we will need to test if the high temperatures and pressures degrade the drugs molecules present in the sample.

Roles and responsibilities:

- Alison Holliday will assist with troubleshooting and method development for gas chromatography-mass spectrometry and solid phase extraction

- To start each day, Madison will have a meeting (~30 minutes) with Alison and the other member of the research group (who will be working on a different project). Results will be reported and discussed and plans for the day will be proposed and discussed.

- Madison will maintain a laboratory notebook that will include regular and complete entries, such that another student could follow her experimental progress. This includes ideas behind experiments, details of experiments (including solution preparation), the location of any electronic data files containing results or analysis, and a summary of results from each experiment. The notebook will be submitted to Alison upon completion of the research project.

- Madison will prepare a brief (<5 page) report to summarize her summer progress on the project.

- A poster would be presented at the Annual Student Scholarship and Creative Endeavors Day in Spring 2019.

Project timetable

Week 1-2: Develop a derivatization procedure for the four different drugs and their metabolites that can all be used in the same sample.

Week 3-4: Develop a solid phase extraction technique that can be efficiently used with all above mentioned drugs.

Week 4-5: Test the effect of autoclaving on the sample.

Week 6-7: Analyze the wastewater for drugs and their metabolites.

Week 8-9: Reanalyze and alter methods as needed.

Week 10: Write report and prepare poster.

Student engagement in discipline-appropriate scholarly research

Analytical chemistry involves the development and testing of new methods or instrumentation to observe and quantify chemical, biological, and physical systems and processes. Forensic chemistry is a subset of analytical chemistry that is devoted to the analysis of substances from a legal setting. Madison will be engaged in forensic analytical chemistry laboratory research that

includes planning and performing experiments involving instrumental methods, analyzing significant amounts of data, and reading the primary literature to contextualize her findings and guide her choice of experimental conditions. Her involvement with forensics will prepare her for graduate school in this field.

Contributions to the Discipline and Opportunities to Share Work

Successful completion of this project may help inform local government or community groups of the status of drug use in the Bethlehem area. The resulting poster may also be presented at the Eastern Analytical Symposium, held in November in Plainsboro, NJ. This symposium frequently exhibits contributions of forensics researchers from the northeast USA.

Project Title: Drug Analysis of Wastewater Using Gas Chromatography-Mass Spectrometry

Student: Madison Pursell

Major: Chemistry

Projected Graduation Date: May 2019

Faculty Mentor: Dr. Holliday, Assistant Professor of Chemistry

On-Campus Housing Request: Yes

I intend to attend graduate school to obtain a Master's Degree in Forensic Science, taking courses to specialize in forensic chemistry. I developed an interest in forensic science when I was young and as a chemistry major, I further developed this interest as I was learning techniques, specifically gas chromatography-mass spectrometry (GC-MS), which is commonly used in the field. After I receive my Master's, I plan to work in the field of drug forensics. Participating in SOAR, and this project specifically, will help me develop skills in instrumental analysis as well as skills that can only be obtained in a lab setting. The benefit of the lab setting being during summer allows me to focus solely on the research that I am doing and also gives me time to develop new methods if previous ones do not work as anticipated. Developing these skills now will prepare me for graduate school as well as a career in forensic science.

By working on this project, I will learn new techniques that will be important for my future education, including solid phase extraction, derivatization, and GC-MS analysis. The solid phase extraction will allow for me to separate drugs and their metabolites from Bethlehem wastewater so that the samples can be purified. Derivatization allows polar molecules that could not typically be analyzed through GC-MS, due to the non-polar GC column, the ability to become non-polar so that they can be analyzed by GC-MS. Through GC-MS analysis of the water samples, we will be able to determine what type and the relative amount of each drug that is present in wastewater. These techniques will all be beneficial in preparing for my future career.

This project also poses potential benefits to the local community. The extent of the drug abuse problem in Bethlehem is likely not known. If the amount of each drug or metabolite in the city's wastewater can be determined, it can assist in truly understanding the severity of the problem in our local community. This can further assist our community in addressing the problem at hand.