Student Members of the American Chemical Society Poster Presentation Event
November 6, 2020 5:30 - 7:00 pm
Stonecipher Lecture Hall

Author: Brooke Underwood*, Courtney LaPointe, Dr. Jeffrey Boles
Contact information: baunderwoo42@tntech.edu

Title: Liquid-liquid extraction and ultraviolet visible spectroscopy methods for distinguishing between hemp and marijuana

Abstract: In December 2018, cannabis containing less than 0.3% tetrahydrocannabinol (THC), otherwise known as hemp, became legalized due to passage of the Farm Bill (1). This creates problems for law enforcement since current presumptive test kits either 1) don't work at all or 2) work somewhat in differentiating between legal and illegal hemp crops. This problem exists because most hemp crops and hemp products contain low levels of THC and the carboxylated form, THCA. Our approach involves the advancement of an efficient, mobile, liquid-liquid extraction (LLE) that provides presumptive, qualitative forensic evidence of the chemical extract of a bud or other plant material. This research is focused on developing a kit that functions in a similar manner to NIK kits, commonly used by law enforcement, where all components of the kit are contained within a bag. The current NIK kit for Marijuana provides a false positive when Hemp is placed in the bag, thus creating the need for a more reliable test (2). The evidence would later be sent to a crime lab for definitive analysis and quantitation of THC by ultraviolet-visible spectroscopy (UV-vis). This research has focused on the utilization of liquid-liquid extraction techniques and commercially available stains. The methods presented are rapid (requiring no more than five to six minutes to complete). The differentiation between two lots of commercially available hemp and seven lots of marijuana obtained from the Cookeville City Police will be presented.

Author: Jonah Ralston*, William R. Carroll
Contact information: jmralston42@tntech.edu

Title: Synthesis of a Terpene: an Abietane-Scaffold

Abstract: Terpenes are isoprene based natural products with a vast range of applications from medical to environmental. They have demonstrated biological activity with a number of protein partners such as JNK3 proteins, topoisomerase, and the ASK3 protein. The synthesis of terpenes poses many challenges due to their complex and specific stereochemistry as well as their volatility, often afford low yielding synthesis. Previously, Cadinane was the target molecule of choice but through prior work and modeling a new scaffold was determined. Using new developments in chemical syntheses, an abietane-like terpenoid backbone is to be synthesized which may be derivatized to obtain a novel terpenoid. Due to the challenges, optimization of these syntheses with design of experiment protocols is used and if appropriate reactions are performed in flow chemical reactors.

Author: Caroline Hunter* and Oana Andreea Cojocaru
Contact information: cahunter42@tntech.edu

Title: Liquid State Pharmaceuticals Based on Aliphatic Dicarboxylic Acids

Abstract:Pharmaceuticals are necessary aspects of everyday life for many people. Unfortunately, pharmaceuticals can also pose dangerous health risks for individuals, as well as side effects, mostly provided by their inherent solid state (e.g., limited bioavailability and aqueous solubility; change in their activity due to polymorphic changes). These issues can be addressed by converting solid-state pharmaceuticals into liquid-state compounds with melting points below body temperature, such as ionic liquids (ILs) and double salt ionic liquids (DSILs). These strategies allow the development of liquid-state pharmaceuticals that will potentially avoid harmful side effects that the solid-state poses while adding dual functionality. Furthermore, a liquid state would provide additional methods of drug delivery, making it beneficial for individuals that are unable to ingest drugs in tablet form. To form liquid state compounds, cation and anion precursors are combined either in a 1:1 ratio (when ILs with two ions of different biological activity are obtained) or in different molar ratios (when DSILs that

can contain three or more ions of different biological activity are obtained). Amines or ammonium salts are used as cation precursors while carboxylic acids or metal carboxylates are used as anion precursors.
This presentation focuses on the synthesis and spectroscopic characterization of new liquid state compounds obtained by combining various pharmaceuticals (e.g., thioridazine, lidocaine, promazine) as cation precursors with aliphatic dicarboxylic acids as anion precursors in different molar ratios.

Author: Devon Cotter* and O. Andreea Cojocaru, PhD
Contact information: dmcotter42@tntech.edu

Title: Synthesis and Solubility Studies of Dual Active Asthma Drugs in Liquid State

Abstract: Patients suffering from asthma and COPD receive treatment in the form of solid-state ingestible tablets or inhalants. Such forms of treatment are not a pervasive solution to those suffering from long term asthma and severe COPD due to the delivery effectiveness of most beta-agonists and corticosteroids such as albuterol and fluticasone (common drugs prescribed for dealing with asthma exacerbation with worsening conditions). Effectiveness of delivery derives from administration (i.e. inhaled medications hardly reach below the larynx of the human body). Thus, the intended effect of the drug is lost amid delivery complications. An alternative method to inhalants that contiguously resolves complications with delivery and effect while mitigating the use of corticosteroids is to administer these drugs in an ionic liquid form. An ionic liquid approach would be especially useful against standard dry powder inhalants (DPIs) as these solid state drugs can exist in multiple crystalline forms (i.e., polymorphism). Polymorphism declines the drug solvation ultimately decimating its bioavailability while converting the drug to less or nonactive forms. Ionic liquids with multiple cations and anions of varying molar ratios balanced by a neutral charge (e.g., one cation and multiple anions, multiple cations and one anion, or multiple cations and anions) are known as double salt ionic liquids (DSILs). When applied to pharmaceuticals, the DSIL approach should increase drug bioavailability (higher aqueous solubility), remove the existence of polymorphic forms, and add multifunctionality to the final drugs (i.e., the pharmaceutical activity of the parent ions is retained). This study investigates the DSIL forming properties of albuterol when combined with ionic forms of over-the-counter non-steroidal anti-inflammatory drugs (NSAIDs) and docusate anion (a known penetration enhancer), as well as the aqueous solubility of the synthesized compounds.

Author: Claire Rust* and Dr. O. Andreaa Cojocaru
Contact information: cerust42@tntech.edu

Title: Solubility of thioridazine double salt ionic liquids in phosphate buffer saline

Abstract: Thioridazine, a member of the phenothiazine drug class, is used as a treatment for the symptoms of schizophrenia and other psychotic conditions. However, this drug has reportedly caused many life-threatening issues including cardiac arrhythmia. This drug is currently manufactured as a solid state drug and its crystalline structure inhibits its ability to function as expected due to lower aqueous solubility as well as its existence in different polymorphic structures. By converting this drug into a liquid form, an ionic liquid (IL) or a double salt ionic liquid (DSIL), new, highly viscous liquid state drugs with new, more desirable properties (e.g., increased aqueous solubility and retained activity) will be obtained.
This presentation focuses on combining various molar ratios of thioridazine, as a cation precursor, with lidocaine cation and docusate anion to create multifunctional DSILs. The two ionic components, lidocaine cation and docusate anion, are added to combat thioridazine's negative side effect of cardiac arrhythmia and to provide the drug with extra delivery options (i.e., transdermal delivery). Three new DSILs were synthesized using the strategies reported in the literature and their aqueous solubility in phosphate buffer saline (pH = 7.4) was investigated.

Author: Courtney LaPointe*, Brooke Underwood, Dr. Jeffrey Boles
Contact information: celapointe42@tntech.edu

Title: A rapid thin- layer chromatography based presumptive test that differentiates between hemp and marijuana

Abstract: The passage of the 2018 Farm Bill, legalizing cannabis containing less than 0.3% THC (Hemp), creates problems for law enforcement. Due to the presence of low levels of THCA and THC present in most commercial hemp crops, law enforcement needs to acquire the ability to distinguish between hemp and marijuana using a presumptive test kit. Our approach involves the development of an efficient, mobile, rapid thin layer chromatography (TLC) kit that provides presumptive (qualitative) forensic evidence of the chemical extract of a bud or other plant material. The evidence would later be sent to a crime lab for definitive analysis of tetrahydrocannabinol (THC) content, the psychoactive compound in marijuana. This research has focused on the utilization of TLC plates along with the spectroscopic and spectrometric identification of resolved cannabinoids. The method presented takes no more than five to six minutes to complete. The successful differentiation between fifteen lots of hemp and seven lots of marijuana will be presented along with spectroscopic and spectrometric identification of resolved cannabinoids.

Author: Bethann M. Oberlander*, Tammy Boles, Bhavya Sharma
Contact information: bmoberland42@tntech.edu

Title: Raman Spectroscopy for the Investigation of Molecules Associated with Human Decomposition

Abstract: The determination of the time since death occurred, or post-mortem interval (PMI), is an important step in death investigations. Currently, the most common approach for determining PMI has been the application of different types of mass spectrometry. Mass spectrometry requires the sample to be in a specific state resulting in sample destruction during the process of acquisition. Raman spectroscopy is a non-destructive technique that is capable of measuring samples in solid, liquid, or gas phases, making it particularly useful in forensic investigations. For this project, three molecules associated with human decomposition and PMI, hypoxanthine, indole, and 3- methylindole were measured with both normal Raman and surface-enhanced Raman spectroscopy (SERS) with gold nanoparticles (AuNPs). Normal Raman was performed for the detection of solid analytes in soil. SERS was performed for the detection of dissolved samples in agarose, layered with soil. All analytes were detected in solid-state mixed with soil as well as in the compounds incubated in agarose and layered in soil. Current work is underway to detect the analytes in the blood of animals resembling humans, notably pigs. Two separate methods will be tested to determine the most accurate and effective way of measuring analyte concentrations in whole blood. Determination of the concentrations of these analytes in bodily systems of animals will help to establish the means for a limit of detection study (LOD) and determine sampling intervals for a longer-term decomposition study as well as ensuring the most ideal animal model is chosen for the study.