DEPARTMENT OF CHEMISTRY

Austin Peay State University

CLARKSVILLE TENNESSEE

The 15th Annual

Undergraduate Research Symposium

Thursday, Nov. 21, 2024

Welcome to the 15th Annual Undergraduate Research Symposium

The Austin Peay State University Department of Chemistry is proud to display the hard work of its research students. The symposium is an opportunity for our students to engage in intellectual conversations with their peers and our community.

The presentations represent the research performed by students involved in CHEM 2941 (Introduction to Research) or CHEM 4941 (Elements of Research). All projects involved research and close collaboration with faculty members. As you are enjoying the presentations, feel free to ask the students questions about their work or what is required to participate in undergraduate research.

CHEM 2940 and 2941 are introduction to research courses focused on student's first experiences with scientific literature, research, ethics, project design and implementation. CHEM 2940/1 courses are designed for students who have completed at least General Chemistry I, but the requirements are at the discretion of the instructor.

CHEM 4941 is an elements of research course that allows students the flexibility and independence needed to learn what is required to thrive in the research world. This research equips students with rigorous critical thinking skills required in industry, graduate programs and professional schools.

CHEM 4990 is a course that allows students to develop an undergraduate thesis. This course requires students to create a report on their completed research and present it to a committee of faculty members.

Faculty Research Biographies

Dr. Allen Chaparadza is interested in technological devices based on solid materials that have certain chemical, physical or electronic properties. Their group is involved in basic research which addresses fundamental issues and challenges affecting materials used in chemical sensors, environmental remediation, biomaterials and metal matrix nanocomposites for structural reinforcement. Current research interests include photoelectrical CO_2 fixing using oxide-based photodiodes, nanostructured materials for biomedical imaging, development of photoreactive semiconductor oxides for anti-biological or chemical decontamination applications, development of sensors for metal ions detection and metal matrix nanocomposites for structural reinforcement.

Dr. Anuradha Pathiranage's primary area of research interest is organic synthesis, especially in medicinal chemistry. She is currently working on several organic chemistry projects. One project involves the synthesis and computational analysis of potential organic UV filters through aldol condensation reaction. The second project is focused on the isolation and characterization of bioactive components of medicinal plants. Her students are currently working on structural analysis and characterization of cannabidiol.

Dr. Carrie Brennan does a wide variety of analytical and materials research! Come see her if you are interested.

Dr. Cody Covington has many research interests in computational chemistry ranging from properties of small molecules to large surfactant and protein systems. He is willing to take on any project, though his current projects are on photoelectron circular dichroism, hydrogen transmission through graphene and the electronic properties of doped tin oxide. Covington also maintains several computer codes, so any students interested in coding can contribute.

Dr. Fred Matthews is interested in Fischer esterification producing hexyl acetates, which are to be identified using bp, refractive index, GLC, GCMS, IR, plus PMR, CMR, GATEDEC, DEPT45, DEPT90, DEPT135, DEPTQ135, COSY, TOCSY, HSQC and HMBC NMR experiments.

Dr. Leslie Hiatt is interested in instrumental and analytical research. Her group is working to develop an assay for the detection of nicotine in electronic cigarettes using electrochemistry. This assay could be used commercially to help small stores demonstrate the quality of their product. Gas chromatography mass spectrometry with nicotine calibration curves is also used to analyze electronic cigarettes. Additionally, liquid chromatography mass spectrometry will be used to analyze carotenoids to aid in the study of fish mating behaviors.

Dr. Meagan Mann's research interests span biochemistry, organic chemistry, toxicology and chemical pedagogy. Her biochemistry subgroup is currently studying effective laboratory experiments for demonstrating toxicological principles. Her organic chemistry subgroup is looking into claims of medical benefits from active components in essential oils. She also collaborates with Dr. Hiatt on the electronic cigarette project. Mann is currently accepting students with strong organic chemistry skills or biochemistry skills.

Dr. Robin Reed's research interests are in protein kinases and proteins that may bind to specific kinases in the cell. These enzymes catalyze the transfer of the γ-phosphate from ATP to specific serine, threonine or tyrosine residues of target proteins. Of particular interest are the cyclic-nucleotide dependent protein kinases, PKA and PKG, and their involvement in signal transduction pathways. One technique used to isolate proteins that bind to PKA or PKG is cAMP-agarose chromatography. Student researchers in his lab have recently verified that one such cAMP-agarose binding protein is the Nucleoside Diphosphate Kinase (NDPK) that is responsible for shifting phosphate groups among various phosphorylated forms of the nucleotides. Reed always seeks energetic student researchers to help him with these projects!

Dr. Lisa Sullivan enjoys making new materials and learning about their properties. If you think it would be cool to explore the entire periodic table, specifically the transition metals, then working with Sullivan would be for you. Her students are investigating a low-temperature synthesis of zirconium tungstate (ZrW_2O_8) which shows isotropic negative thermal expansion. Prepared nanoparticulate ZrW_2O_8 will be incorporated into a polymer thin film to give a composite material that has controllable thermal expansion. Her students are also investigating a novel synthetic preparation of nanoparticulate silver and studying the antimicrobial efficacy of prepared samples.

List of Presenters

Analytical Chemistry

#1. Jamaya Moore
Co-author: Carrie Brennan

Optimization of an HPLC Method for Simultaneous Analysis of Pesticides and Antibiotics in Environmental Water Samples

Environmental water quality is of growing concern associated with agricultural and drug metabolite pollution. Even at low concentrations, herbicides, pesticides, and antibiotics can negatively impact the health of humans and local wildlife. While many methods exist for the detection of either herbicides/pesticides or antibiotics, there is no method available that can detect both simultaneously. This research focuses on developing a single HPLC method to detect and quantify the herbicides glyphosate, 2,4-dichlorophenoxyacetic acid (2,4-D), and 2,4-D methyl ester and the antibiotic ciprofloxacin. Once the assay is developed, it will be used to process samples from local bodies of water. While ongoing instrument maintenance has enhanced peak retention times for most analytes, some noise remains, particularly with the new glyphosate analyte.

#2. Kamiliya Aumiller
Co-author: Leslie Hiatt

Identifying Caffeine Using Gas Chromatography Mass Spectrometry

Caffeine is a methylxanthine stimulant chemical used in many over-the-counter medicinal drugs containing acetaminophen. The goal of our research was to examine and quantitate caffeine in comparison to the labelled quantities of caffeine in over counter bottles of Excedrin. Chromatography parameters were altered to develop a robust method of detection. A calibration curves was developed by diluting caffeine in acetone at concentrations of 0.5 to 30.0 ppm. Various over-the-counter drug tablets (n=6, labelled as 65 mg/pill) were ground up using a mortar and pestle and filtered (11 μm) using acetone. The analytes were diluted further and syringe filtered (0.45 μm). Analysis demonstrated a percent difference between the stated label and GCMS determined amount of caffeine to be between 134% and 33% per pill.

#3. Holly Garcia
Co-author: Leslie Hiatt

Cracking the Capsule: GCMS Analysis of Ibuprofen

Ibuprofen is a common nonsteroidal anti-inflammatory drug (NSAID). The purpose of this research is to develop the methodology and instrumental parameters to evaluate Ibuprofen using the Gas Chromatography Mass Spectrometer (GMCS). The analysis of ibuprofen laid the foundation for the comparison of experimentally induced degradation of premium-brand and generic prescription drugs. With standard solutions ranging 1000-7500 ppm, varying GCMS methods were evaluated to develop an analysis that allowed the quantitative analysis of ibuprofen. The premium brand ibuprofen and generic brand ibuprofen, respectively, were ground into a fine powder using mortar and pestle. The capsule and filler were filtered using filtration paper and rinsed with methanol solvent before analysis by GCMS. The calibration curve was used to quantitate the amount of ibuprofen in each pill, which was stated to contain 200 mg of ibuprofen. “Major” premium brand ibuprofen expired in 2008 and was analyzed to contain 48.8 mg ibuprofen per capsule, while the generic “Walgreens” brand was determined to contain 107.7 mg ibuprofen per pill. The analysis resulted in a 24% and 54% recovery for the expired brand and new ibuprofen respectively. Future experiments will result in method improvement and analysis of premium brand and generic brand products over varying drug types.

#4. Arianna Banta

Co-authors: Carrie Brennan, Leslie Hiatt

Identifying Metal Concentrations in Cocoa

This research aimed to create a reliable method to extract, measure, and compare the quantity of metals between the different components of the cocoa bean, such as cocoa powder, the cocoa bean shell, and the inner cocoa nibs. The calcium concentration present in cocoa beans sourced from Columbia found in prior literature was used as a basis for this research. A dry ashing method was used to analyze the cocoa samples. This method involved heating samples in crucibles at 500 °C in a furnace until all the cocoa was ashed. The mass of the ash was measured every 30 minutes to ensure all organic matter was burned off the sample. The ash was then dissolved in nitric acid and filtered. Afterward, the calcium concentration was assessed in each sample using flame atomic absorption spectroscopy. Multiple dry-ashing experiments were conducted. The first experiment tested the precision of the dry ashing process. Later experiments improved the process and examined the differences in calcium levels of the different parts of the bean. It was found that the shell of the cocoa bean held the most calcium as compared to other components of the cocoa bean. The results of the dry ashing experiments demonstrate promise as an accurate and precise technique for metal analysis as compared to published literature methods.

#5. Gary Hendricks

Co- authors: Leslie Hiatt, Carrie Brennan

Wet Digestion of Cocoa Powder to Determine Metal Concentration

Over the past three years, Consumer Reports has highlighted elevated levels of toxic metals, including lead and cadmium, in commonly consumed chocolate products. This project aims to establish a wet digestion method to accurately determine the heavy metal contents in chocolate products. To find a suitable method, calcium concentration was investigated, due to its lesser toxicity than lead or cadmium. Wet digestion is a method that breaks down the organic molecules to isolate the metal contents. Small samples of Trader Joe's cocoa powder were treated with a combination of nitric acid, perchloric acid, hydrogen peroxide, and in some cases lipase. These acidified samples were heated using heating mantles, with slow additions of hydrogen peroxide. The first technique utilized the addition of nitric acid, perchloric acid, and hydrogen peroxide, while the second technique utilized lipase as a pretreatment option before adding nitric acid, perchloric acid, and hydrogen peroxide. All samples were analyzed using external calibration and atomic absorption spectroscopy. The first technique produced four clear colorless products, that were slightly below expected values based on peer reviewed articles. The second technique produced three clear but yellow products, which were in the range of expected values. Wet digestion provides a foundation for future studies of metals in chocolates. With minor adjustments this method can be used to accurately determine the amounts of more toxic metals such as lead or cadmium.

#6. Jackson Brown
Co-authors: Bohdan Mahlovanyi, Roksolana Pasternak, Michał Golena, Dr. Yaroslav Shpotyuk Dr. Andriy Luchechko, Dr. Jozef Cebulski

Photoluminescence and optical transmission of borate glasses doped with rare earth metal ions

The optical transmission, luminescence excitation, and photoluminescence properties of borate-based glasses doped with rare earth metal ions have been investigated. The borate glasses are of two matrixes, $(B_2O_3)_{58-X}$-$(CaO)_{20}$-$(Li_2O)_{20}$-$(Bi_2O_3)_2$-$(MO)_X$ and $(B_2O_3)_{60-X}$-$(ZnO)_{10}$-$(SrO)_{10}$-$(CaO)_{10}$-$(MgO)_{10}$-$(MO)_X$, where MO is the rare earth metal oxide (M = Dy, Pr, Eu) and X is the concentration in the total composition of the rare earth metal oxide. Each glass was synthesized using the melt quenching technique and was polished to obtain high optical quality. The photoluminescence studies showed that the optimal concentration of Dy is 0.75% as any concentration higher causes luminescence quenching. For Dy, the photoluminescence spectra shows two peaks with one correlating to blue light and one correlating to yellow light. For Pr-doped glass, there is one band in the orange light wavelength under λ_{exe}= 446 nm excitation. For Eu-doped glass, there are two bands with one of each in the yellow light and the orange light regions under λ_{exe} = 393 nm excitation. When Pr and Eu are co-doped with Dy in equal concentrations, each demonstrate two bands: one in the blue light region and one in the yellow light region. While not all combinations were successful in promoting a white light optical emission, when the glass was doped with Dy and co-doped with Pr and Eu in equal amounts, it provided two bands which resulted in white light.

#7. Aidan Milam

Co-authors: Jiri Jancalek, Stanislav Slang, Michal Kurka

Characterization of Chalcogenide Glasses with Increasing Indium Content

Chalcogenide glasses (ChGs) are amorphous materials made primarily from chalcogen elements (Group 16), often combined with other elements like germanium and arsenic. These ChGs are known for having unique optical properties, including high refractive indexes and a wide infrared transparency range, making them useful in photonics and optical applications. This study investigates the film thickness, optical bandgap, refractive index, and chemical structure of ChGs with increasing indium content of $Ge_{25-x}In_xSe_{75}$ amorphous thin films by 0, 2.5, 5, 7.5, and 10% through solution processing. The bulk glass was synthesized using pure elements with the melt quenching technique, and thin films were created by spin coating the ChG solution on chemically cleaned microscope slides with three to four samples that were annealed at 60, 120, 180, and 210 ^oC respectively. These thin films were characterized by UV-Vis, FTIR, Raman spectroscopy, energy dispersive spectroscopy (EDS), wet etching, and scanning electron microscopy (SEM). The practical applications of these thin films were tested using holography, electron beam lithography (EBL), and hot embossing. With increasing indium content, samples showed greater thickness contraction, larger optical bandgaps, and higher refractive indices. Similarly, higher annealing temperatures led to thickness contraction, reduced optical bandgaps, and increased refractive indices.

Organic and Medicinal Chemistry

#8. Sarai Faulkner
Co-authors: Bailey Sheddan, Meagan Mann

Title: Synthetization and Characterization of Epoxy-modified ursolic acid

Ursolic acid is a naturally occurring pentacyclic terpenoid acid found in various medicinal herbs and plants. Numerous studies have highlighted its biological activities and medicinal properties, including hepatoprotective effects. Research has shown that when metabolized, ursolic acid transforms into several epoxy-modified derivatives. This project aims to evaluate the hepatoprotective efficacy of epoxy-ursolic acid in the treatment of alcohol-related liver disease. Epoxy-ursolic acid was synthesized from ursolic acid through an epoxidation reaction. The crude product was purified using column chromatography, and the purified epoxy-ursolic acid is undergoing identification and characterization by nuclear magnetic resonance (NMR) spectroscopy. Future work will focus on further characterization of the epoxy-ursolic acid product and conducting biological assays.

THANK YOU FOR JOINING US!

If attending this research symposium increased your interest in participating in undergraduate research, please speak with your advisor and faculty members.

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