

# ABSTRACTS

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Jacobs Science Building  
April 28, 2017  
11:30am - 3:30pm

Department of Chemistry  
University of Kentucky  
Lexington, KY 40506



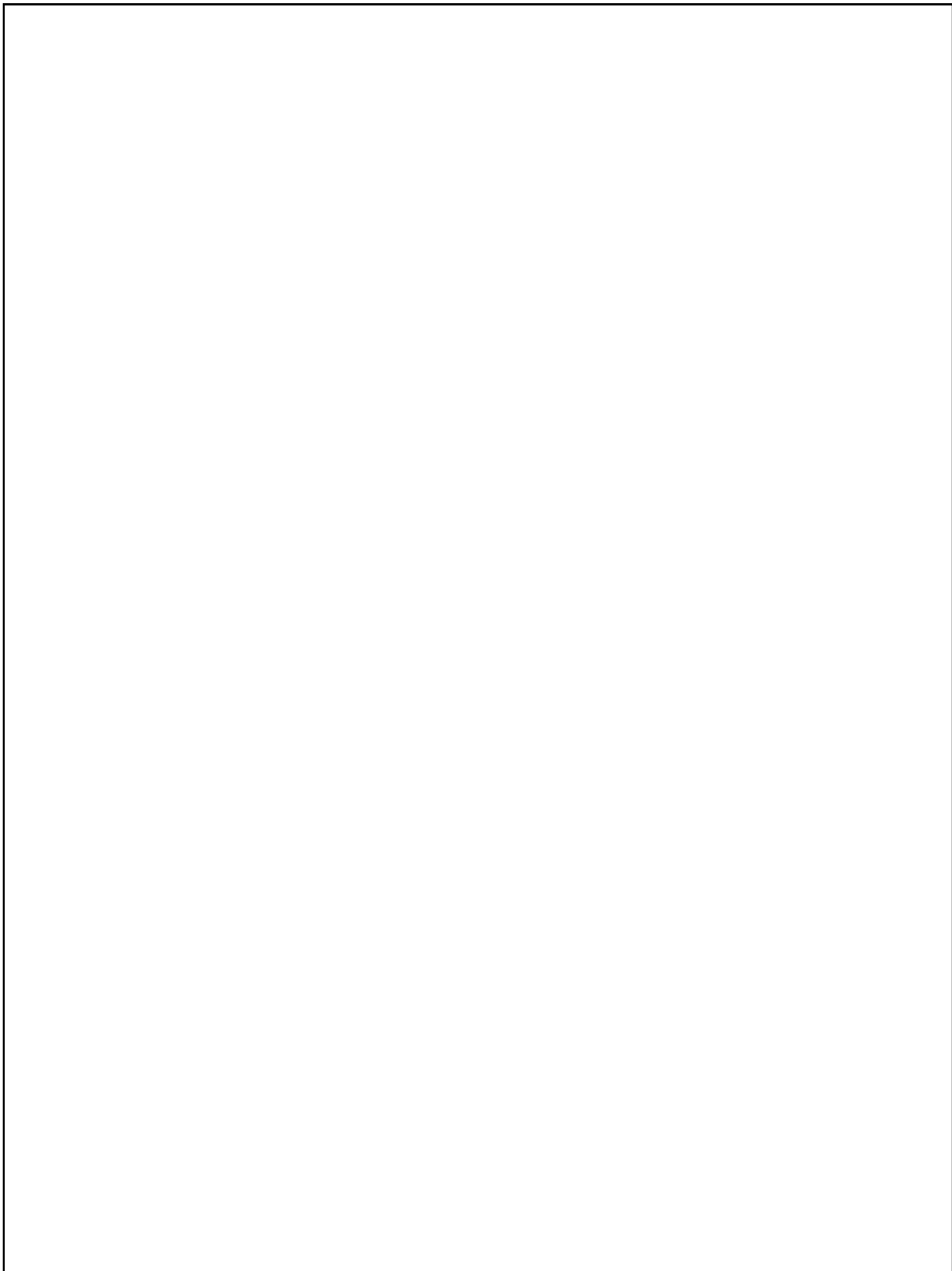
# 1

## **DIFFERENTIATION OF ISOMERIC HEPARAN SULFATE USING MASS SPECTROMETRY, TANDEM MASS SPECTROMETRY AND PRINCIPLE COMPONENT ANALYSIS.**

**John Attelah, Junior, Chemistry, Berea College**

**Isaac Agyekum, Chemistry, The University of Georgia**

Glycosaminoglycans (GAGs) are complex polysaccharides, expressed at the cell surface and in the extra-cellular matrix, which comprise the carbohydrates portion of proteoglycans and are found in a variety of organisms ranging from bacteria to humans. GAGs participate in a number of significant biological processes, such as cell-cell and cell-matrix signaling at the origin of a variety of physiological and pathological functions such as embryonic development, cell adhesion, the regulation of biochemical pathways, cell growth and differentiation, homeostasis, and the mediation of inflammatory reactions. They have also been implicated in the initial step of some pathogenic infections and have been observed to undergo some alteration in some tumor growth. There are different types of GAGs which include Chondroitin Sulfates(CS), Dermatan Sulfates(DS), Keratan Sulfates(KS), Heparin and Heparan Sulfates(HS). Since a better understanding of structural, and binding properties of HS is required for development of HS mimetic, and possible new glycotherapeutics, increasing interest in protein-carbohydrate interactions is accompanied by challenging demand for viable, accurate and high-throughput methodology for their characterization. Therefore, the objective of the project was to use Mass spectrometry, Fourier Transform Mass Spectrometry and Principal Component Analysis (PCA) to diagnostically distinguish between isomeric Heparan Sulfate Glycosaminoglycans.



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## AMMUNITION DIFFERENTIATION BY ICP-AES ANALYSIS OF GUNSHOT RESIDUE

Chris Barbera, Senior, Chemistry, Hanover College

Craig Philipp, Chemistry, Hanover College

Most gunshot residue, or GSR, testing is a simple positive or negative response to the presence of GSR. There are not many techniques that easily give qualitative and quantitative data of GSR limiting the information that can be used. We used ICP-

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## INVESTIGATING THE IN SILICO OPTICAL CHARACTERISTICS OF TRIALKYLSILYLETHYNYL PENTACENE DERIVATIVES USING GW-BSE CALCULATIONS

Kristen Brooks, Senior, Chemistry, University of Kentucky

Karol Jarolimek, Chemistry, University of Kentucky

Chad Risko, Chemistry, University of Kentucky

Solar cells convert energy from light into electricity via the photovoltaic effect. The theoretical power conversion efficiency of conventional inorganic solar cells using a p-n junction is limited by the Shockley-Queisser Efficiency Limit; however, organic semiconductors which utilize singlet fission have been found to exceed this limit. Two such organic semiconductors are 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS pentacene) and 6,13-bis(triethylsilylethynyl) pentacene (TES pentacene), which respectively adopt two-dimensional brickwork and one-dimensional slipped-stack packing arrangements. Despite similarities in the structures of these two molecules, their performances as organic semiconductors vary significantly as a result of their packing arrangements. In this experiment, the in silico optical characteristics of brickwork and slipped-stack polymorphs of both TIPS pentacene and TES pentacene were calculated using GW approximations coupled with BSE (Bethe-Salpeter Equation). By comparing these optical characteristics, the effects of packing arrangement on organic solar cell performance may be further determined.

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## EFFECTS OF SURFACE MODIFICATION ON THE PHOTOLUMINESCENCE QUANTUM YIELD OF METHYLAMMONIUM LEAD IODIDE PEROVSKITES

Jillian Cramer, Senior, Chemistry, University of Kentucky

Kenneth Graham, Chemistry, University of Kentucky

Methylammonium lead iodide perovskites have been shown to be an effective light-absorbing active layer in solar cells, but suffer from low stability and inconsistent performance due in part to defects at the surface. These defects can lead to “trap states,” inhibiting the transport of charge carriers across the device and increasing unwanted nonradiative decay. However, surface modifiers, such as phosphonic acids, carboxylic acids, thiols, trichlorosilanes, amines, and zwitterions studied here, may improve the surface chemistry and mitigate the formation of trap states. Ideally, the surface modifiers strongly bind to the lead iodide perovskite and improve the performance and stability of the device.





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## KINETIC INVESTIGATION OF RING-OPENING POLYMERIZATIONS USING A BIMETALLIC CATALYST

Benjamin Demor, Senior, Chemistry and Biochemistry,

Rose-Hulman Institute of Technology

Stephanie Poland, Chemistry and Biochemistry, Rose-Hulman Institute of Technology

Research on biodegradable polymers is of interest as they have many applications in the biomedical field. Two such polymers that can be used for these applications are polytrimethylene carbonate and polylactide. In this study, a previously developed and investigated bimetallic magnesium catalyst was used for a catalytic ring-opening polymerization (ROP) of trimethylene carbonate (TMC) and lactide. A kinetic investigation using IR spectroscopy and an attempt at  $^1\text{H}$  NMR spectroscopy found that the catalyzed reaction occurs at a faster rate than previously believed. With the use of  $^1\text{H}$  NMR to monitor reaction conversion, it was shown that the ROP of lactide with this catalyst is inefficient with very long reaction times. The development of these kinetic investigations for the two cyclic monomers will be discussed.



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## THE SYNTHESIS AND SPECTROSCOPY OF NINE BENZIL-BASED LIGANDS AND THEIR PALLADIUM (II) COMPLEXES

Eric Dobias, Sophomore, Chemistry, Thomas More College

Tyler Green, Chemistry, Thomas More College

Daniel Esterline, Chemistry, Thomas More College

Diimine ligands have various uses in pharmaceuticals, industry, and major biological processes. The purpose of this research was to synthesize the ligands N,N'-di(4-bromophenyl)-1,2-diphenylethane-1,2-diimine and N,N'-di(4-methoxyphenyl)-1,2-diphenylethane-1,2-diimine as well as six analogues using different aniline reagents. The aniline compounds contain different substituents in varied positions on the benzene ring, which may impact the overall viability of the reactions. Benzil and toluene-sulfonic acid were reacted with the appropriate aniline starting material. The products have been characterized by <sup>1</sup>H NMR Spectroscopy, Infrared Spectroscopy, and Gas Chromatography Mass Spectrometry. Results indicate that the original two ligands were successfully synthesized.

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## EXPERIMENTAL DESIGN OF RING OPENING POLYMERIZATION OF CYCLOHEXENE OXIDE BY SOLID CO<sub>2</sub>

Taylor Downs, Senior, Chemistry, Rose-Hulman Institute of Technology  
Dr. Stephanie Poland, Chemistry, Rose-Hulman Institute of Technology

Carbon dioxide and epoxide coupling to yield polycarbonates has been a major focus in plastics research since its discovery in 1969 by Shohei Inoue. The downfalls to using this original method in undergraduate laboratories involve unsafe reaction conditions because of the high pressures of CO<sub>2</sub> required and the need for costly stainless steel reactors. Many advancements towards making this synthesize less hazardous include using ambient reaction temperatures, operating at 1 atm pressures in the reaction vessels, and utilizing less reactive epoxides. All these changes lead to the greener synthesis of polycarbonates that can be used in electronics, consumable goods, optical media, and the automotive and medical industries. This study focuses on creating a laboratory experimental design to introduce undergraduate students to catalysis, polymerization, and green chemistry. Using techniques used in a previous Organic Chemistry lab at RHIT, carbon dioxide and air-stable cyclohexene oxide were coupled using various transition metal catalysts and cocatalysts in a plastic centrifuge tube. The products were analyzed using <sup>1</sup>H NMR as well as FT-IR spectroscopy. Three (salen)MCl catalysts (M = Co<sup>3+</sup>, Al<sup>3+</sup>, Cr<sup>3+</sup>) were studied to determine which catalyst showed the highest coupling activity. This seminar will detail the optimization route taken toward the goal of successfully producing poly(cyclohexene carbonate) under these restricted conditions.



**SYNTHESIS OF BENZO[b][1,4]THIAZINE-6-CARBOXAMIDE DERIVATIVES AS NOVEL ANTI-EPILEPTIC AGENTS****Abigail Florence, Senior, Chemistry, University of Kentucky**Adam McCluskey, Chemistry, University of Newcastle, AustraliaAndrew Lin, Chemistry, University of Newcastle, Australia

Epilepsy is a neurological disorder that results in frequent seizures, which can lead to a poor quality of life. This disease occurs due to the rapid release, via exocytosis, of neurotransmitter within the brain. It is believed that by being able to slow down the number of vesicles each neuron recycles, the number of seizures within an individual can be reduced or eliminated. A screening of a library of 17,000 compounds showed that benzo[b]thiazine-6-carboximide 1 displayed anti-epileptic activity. A library of compounds was synthesized to establish the exact structure to activity (SAR) relationship of the original compound to the protein interactions. The first key reaction made up the first library of compounds and involved the Knoevenagel condensation, which reacts aldehydes and ketones together in the presence of a weak base. The second key reaction was N-alkylation, which binds an aliphatic amine with a secondary alkyl halide to make up the second library of compounds. The third, and final, reaction was amide coupling, which binds a carboxylic acid with an amine to make up the final library of compounds. All of the compounds for each library have been synthesized and are awaiting an evaluation of biological activity at both Children's Medical Research Institute in Sydney, Australia and Calvary Mater Hospital in Newcastle, Australia.

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**ALGAE-**

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**PHOTOCATALYTIC REDUCTION OF CO<sub>2</sub> ON -Fe<sub>2</sub>O<sub>3</sub>/K<sub>2</sub>O  
HETEROSTRUCTURE USING SOLAR ENERG**

**Kayvon Ghayoumi, Senior, Chemistry, University of Kentucky**

Ruixin Zhou, Chemistry, University of Kentucky

Muthu Gnanamani, Chemistry, University of Kentucky

Kenneth Graham, Chemistry, University of Kentucky

Marcelo Guzman, Chemistry, University of Kentucky



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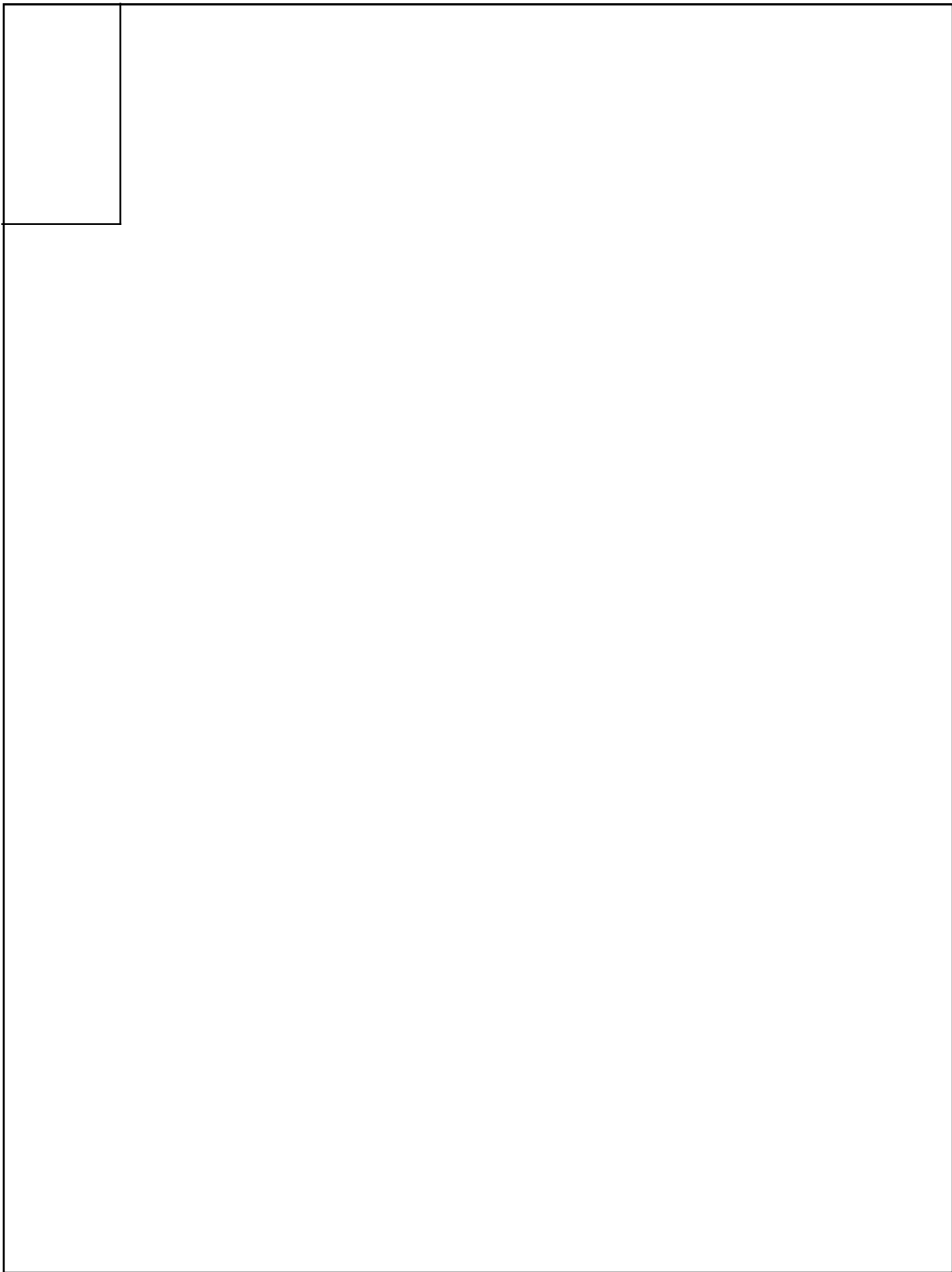
**MTOR SIGNALING IN BRAIN OF A UNIQUE RAT MODEL OF  
PARKINSON DISEASE**

**Sarah Goebel, Senior, Chemistry, University of Kentucky**

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**COMPARISON OF SUBSTRATE BINDING TO A  
HYPERTHERMOPHILIC VS. A MESOPHILIC FLAVOENZYME**





**CARBON BASED CATALYSTS FOR CO<sub>2</sub> REDUCTION****Sidney Herrell, Senior, Chemistry, University of Kentucky**Namal Wanninayake, Chemistry, University of KentuckyDoo Young Kim, Chemistry, University of Kentucky

Significant buildup of greenhouse gas in the environment is a global issue due to the increasing use of fossil fuels. Therefore, the electrochemical reduction of carbon dioxide using renewable energy is important to reduce the anthropogenic CO<sub>2</sub>, which is one of the major contributors to the greenhouse effect. The search for an efficient and durable catalyst for the electrochemical reduction of CO<sub>2</sub> is an active area of research because of the advancements it can lead to in the science and technology of energy conservation and environmental remediation. The electrochemical reduction of CO<sub>2</sub> is dependent on an effective catalyst that reduces the overpotential of the reaction, is selective toward desired products, is durable, and finally, a catalyst that suppresses the hydrogen evolution reaction which occurs during the same potential region and competes with CO<sub>2</sub> reduction process.<sup>1</sup> Development of suitable catalysts for this process, however, is challenging due to the lack of understanding of the catalytic process and limited number of efficient and robust catalysts. Recently, it has been shown that nitrogen-doped carbon shows a great promise towards electrocatalytic reduction of CO<sub>2</sub>. N-doped carbon-based mat b ] mat ased mat b ] m

**ELECTROLESS PLATING ON PLASTICS****Braxton McFarland, Senior, Chemistry, University of Kentucky**

Electroless copper plating is a process similar to plating from a galvanic cell, but does not require an external energy source. The auto catalytic reaction occurs in a plating bath and results in a metal layer plated on top of a substrate. A plating bath is comprised of a reducing agent, complexant, stabilizer and ion source. The electroless method often involves plating metal onto other metal substrates, but also has the capability of plating metal layers on to plastics. We have determined an effective electroless plating process using nonmagnetic materials suitable for an electromagnetic coil as a 3-d printed circuit.

**AB9 ESTERS – SYNTHESIS AND CHARACTERIZATION****Ryan Melody, Senior, Chemistry, University of Kentucky**David Atwood, Chemistry, University of Kentucky

Bidentate dithiol 2,2'-(isophthaloylbis(azanaediyl)bis(3-mercaptopropanioc acid)) (Trade names: ABDTH2 or AB9) is a chelating agent of interest due to its high affinity for heavy metal ions in solution and compatibility with silica attachments. Characterization of magnetic nanoparticle coupling and physical properties has been documented, but due to the complete insolubility of AB9, crystallization has proven unsuccessful.

The purpose of this research project is to synthesize the methyl (ME-AB9) and ethyl (EE-AB9) esters of AB9 and characterize both the complexed and un-complexed structures associated with each ester. Characterization will be performed through techniques such as Infrared Spectrometry, H1-NMR, TGA, DSC, and various crystallization techniquTG

**EFFECTS OF THE WATER CONTENT IN LEAD ACETATE ON MORPHOLOGY AND PV PERFORMANCE OF METHYLAMMONIUM LEAD HALIDE PEROVSKITES**

**Thuy Nguyen, Senior, Chemistry, University of Kentucky**

Kenneth Graham, Chemistry, University of Kentucky

So Min Park, Chemistry, University of Kentucky

Inorganic perovskites have made a breakthrough in solar cells for lower cost and high performance compared to the mass produced silicon solar cells. Due to the difficulties during the fabrication process, reproducibility in these type of cells is relatively poor. Specifically, planar heterojunction methylammonium lead iodide (MAPb3I) perovskite solar cells are highly sensitive to air, annealing time, solvent, and various methods of fabrication. Which lead to the investigation of the effects from purity, brand, and water content of the lead acetate trihydrate, Pb(Ac)<sub>2</sub> precursor on the performance of the PV cells. Although, the lead acetate photoluminescence properties and external quantum efficiency in the sub-bandgap region increase with increasing purity; its performance is often lowered due to other factors. While determining the appropriate amount of water content in the lead acetate had a significantly positive effect on the PV performance and morphology of the films compared to the commercially bought and the dehydrated forms. Optimization of the effects of lead acetate has the potential for as a controllable, reproducible precursor for MAPb3I perovskite solar cells.



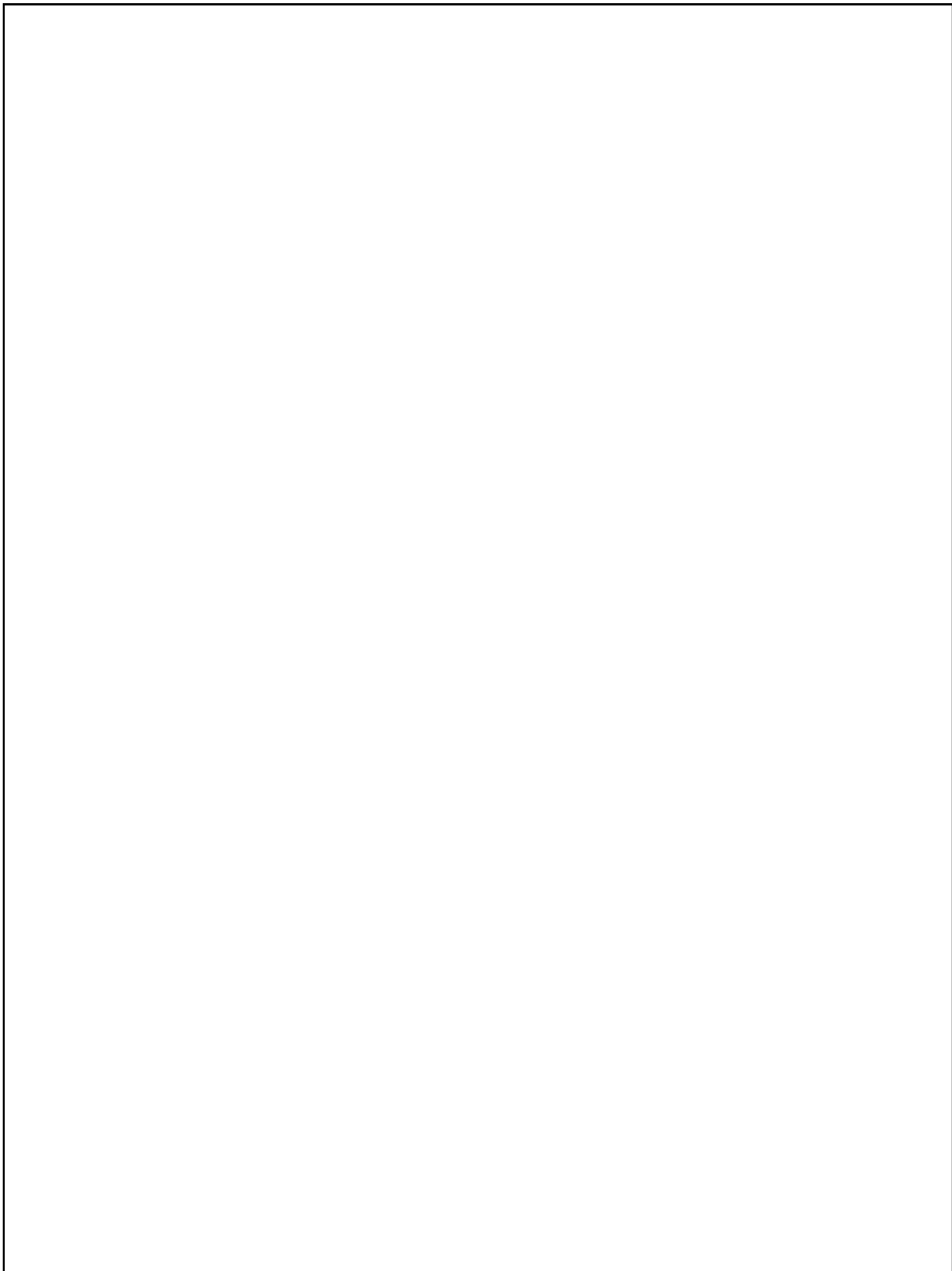
**LAND USE HISTORY, SOIL CHARACTERIZATION AND INVASIVE SPECIES IN THE BEREA COLLEGE FOREST.****Savannah Osborne, Senior, Chemistry, Berea College**

Berea College manages about 9000 acres of forest land that is a valuable part of student life and learning at the college, and is listed on the National Register of Historic Places. The first College Forester was Silas C. Mason (1897-1908), who began land acquisition with his own funds. Most of the newly purchased land was abandoned logged-over land,



**IMPROVED MICROWAVE DIGESTION METHODS FOR BONE ASH AND PORTLAND CEMENT****Amy Rice, Senior, Chemistry, Thomas More College**Kelsey Kaht, Chemistry, University of LouisvilleWilliam Wetzel, Chemistry, Thomas More CollegeChrista Currie, Chemistry, Mount Saint Joseph University

In the early 2000s, a crematorium in Georgia unethically disposed of deceased bodies and provided families with cement in place of authentic cremated remains. Since that time, a variety of methods have been explored to differentiate human cremated remains from other materials. Previous work in our lab has been directed at using two certified reference materials, Bone Ash (NIST 1400) and Portland Cement (NIST 634a), as a model for human cremated remains and other (non-cremated remains) materials. Bone Ash or Portland Cement were dissolved in nitric acid and hydrogen peroxide using microwave-assisted bsa t itric acid



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## IRON-CATALYZED SUBSTITUTION OF ALCOHOLS

Julie Simon, Sophomore, Chemistry, Indiana University

Paul Marcyk, Chemistry, Indiana University

Silas Cook, Chemistry, Indiana University

Alcohols are attractive electrophiles for alkylation as they are widely available, stable and easy to prepare. The Cook group has developed a novel catalytic system to activate alcohols for substitution with nitrogen and arene nucleophiles. My research involves using this system for the activation of alcohols substitution reactions with oxygen and sulfur. Intramolecular substitution with oxygen was successful, but the product underwent undesired Friedel-Crafts Alkylation. Future work will involve adding electron-withdrawing groups in order to deactivate the product from this side reaction. Intramolecular substitution with sulfur has not yet been attempted. Future work will involve identifying a suitable protecting group to synthesize the starting material and attempting the intramolecular substitution.

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**DIFFERENCES IN THE MEMBRANE EXPRESSION OF GPR39 IN THE PRESENCE AND ABSENCE OF ZINC IONS**

**Kimberly Stevens, Senior, Chemistry, University of Kentucky**

Mark Lovell, Chemistry and Sanders-Brown Center on Aging, University of Kentucky

**PREDICTION OF HYDROXYLATION RATE CONSTANTS FROM MOLECULAR STRUCTURE BY CHEMINFORMATICS METHODS WITH COMPUTATIONAL NEURAL NETWORK**

**Darin Vaughan, Junior, Chemistry and Mathematics, Morehead State**

Pharmaceutical drug discovery and design has always been a complicated and time consuming process, especially for purely experimental chemists. This study presents a highly interdisciplinary approach to solving difficult problems in drug discovery through cheminformatics.

Quantitative structure-activity relationship models are a multiple linear regression technique for aiding in predicting certain properties of compounds, such as the relationship between the chemical structure of an enzyme inhibitor and its biological activity. To explore the strength and utility of QSAR methods, a model was developed relating three classes of structure descriptors for a set of unsaturated hydrocarbons which undergo hydroxylation reactions to accurately predict  $k_{OH}$  rate constants. To aid in the advancement of novel and promising technology, computational neural networks (commonly named Artificial Neural Networks) were employed for producing a predictive learning model which resulted in exceptionally low error.

This technique provides a strong measure of confidence for scalability into more complex molecular relationships such enzyme reaction rates which are important for Michaelis-Menten dynamics. The time saving benefit of QSAR and cheminformatics in general is that enzyme assays and extensive reaction spectroscopy are not necessary to determine rate constants. Reaction dynamics may be simulated entirely in silico using such a multidisciplinary approach as this. Combining relatively accessible methods from computer and data science, quantum computational chemistry, applied mathematics, and organic and pharmaceutical chemistry, cheminformatics provides the opportunity for people from any discipline to enter an exciting field.

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