# 2025 Undergraduate STEM Poster Symposium



Friday, August 1, 2025

10 AM - Noon

**Burge Union** 



### Featuring the following programs:

### Chemistry NSF-REU Program (CHE-2349329)

A Summer Experience for Undergraduates Integrating Research, Education, and Career Development in an Interdisciplinary Environment

### **Chemical & Petroleum Engineering NSF-REU Program (EEC-2243816)**

IDEA Incubator for Porous Materials: Integrating Discovery, Engineering and Art

NSF Engineering Research Center EARTH (Environmentally Applied Refrigerant Technology Hub) (EEC- 2330175)

FROST: Fostering Research in Sustainable Technologies

Kansas NSF EPSCoR ARISE REU Program (EPSCoR - 2148878)

Building Pathways to Community Disaster Resilience

### **Pharmaceutical Chemistry Department**

Summer Undergraduate Research Program

Financial and Logistical Support for the Symposium provided by the Madison and Lila Self Graduate Fellowship Program

### Session 1 10:00 AM - 11:00 AM

### Click presenter's name to view poster titles and abstracts

Poster	Presenter	Home Institution	REU Program
P1	<u>Aubrey Brown</u>	Carthage College	Chemistry
Р3	Raina Fair	University of Kansas	Chemistry
P5	Austin Groth	Midwestern State University	Chemistry
P7	Patryk Hupert	University of Kansas	Chemistry
P9	Jamie Neumann	University of Wisconsin Eau Claire	Chemistry
P11	<u>Jermiah Polk</u>	Abilene Christian University	Chemistry
P13	Landon Scott	Baker University	Chemistry
P15	Lily Tackett	University of Kansas	Chemistry
P17	Karissa Wilson	University of Kansas	Chemistry
P19	Joshua Burns	University of Kansas	EPSCoR
P21	Hannah Gideon	Fort Hays State University	EPSCoR
P23	Emily Greer	Kansas State University	EPSCoR
P25	David Hipp	University of Illinois Urbana-Champaign	EPSCoR
P27	Joseph Schauwecker	Mississippi State University	EPSCoR
P29	Camille Taylor	Mississippi State University	EPSCoR
P31	<u>Fayrouz Zeidan</u>	Louisiana Tech University	EPSCoR
P33	Stephanie Dücker	Washington & Lee University	FROST
P35	Alborz Nasseri	Northern Illinois University	FROST
P37	Adam Smith	Arizona State University	FROST
P39	<u>Cameron Burns</u>	University of Wyoming	IDEA
P41	Morgen Keller	University of Kansas	IDEA
P43	<u>Dylan Maloney</u>	University of Kansas	IDEA
P45	<u>Pritam Ray</u>	University of Kansas	IDEA
P47	Ananya Saravana	Washington State University	IDEA
P49	<u>Isaiah True</u>	University of Kansas	IDEA
P51	Jake Ferguson	University of Kansas	Pharm Chem
P53	Hamza Habib	Wesleyan University (CT)	Pharm Chem
P55	Zach Logan	Southwestern University	Pharm Chem
P57	Jason Meschke	University of Kansas	Pharm Chem
P59	<u>Udita Shah</u>	University of Kansas	Pharm Chem
P61	Monica Whalen	University of Kansas-Wichita	Pharm Chem

# Session 2

### 11:00 AM - Noon

### Click presenter's name to view poster titles and abstracts

Poster	Presenter	Home Institution	REU Program
P2	Ashleigh Caldwell	Murray State University	Chemistry
P4	Ellison Gee	University of Kansas	Chemistry
P6	Autumn Harris	Langston University	Chemistry
P8	Spencer Moffitt	Oberlin College	Chemistry
P10	Daisy Orozco	MidAmerica Nazarene University	Chemistry
P12	<u>Keimarya Rivera</u>	Oglethorpe University	Chemistry
P14	Brandon Sikes	Washington University in St. Louis	Chemistry
P16	William Viator	Louisiana Tech University	Chemistry
P18	Nathan Binshtok	University of Kansas	EPSCoR
P20	Ryan Corrigan	University of Kansas	EPSCoR
P22	Matthew Goodman	University of Kansas	EPSCoR
P24	Monique Haynie	University of Kansas	EPSCoR
P26	King Nguyen	Wichita State University	EPSCoR
P28	Aneesh Sivakumar	Kansas State University	EPSCoR
P30	Nicholas Thompson	Kansas State University	EPSCoR
P32	Khue Do	University of Georgia	FROST
P34	Kirshaun McGhee	Delaware State University	FROST
P36	Nicholas Romano	Texas A&M University	FROST
P38	<u>Henry Bair</u>	University of Kansas	IDEA
P40	Oscar Gutierrez	University of Houston	IDEA
P42	<u>Tej Maheshwari</u>	Brown University	IDEA
P44	<u>Tifiani Palm</u>	University of Tulsa	IDEA
P46	Anna Rosu	University of Wisconsin-Madison	IDEA
P48	William Steere	University of New Hampshire	IDEA
P50	Alan Bernstein	Middlebury College (VT)	Pharm Chem
P52	Adriana Gallegos	University of Kansas - Wichita	Pharm Chem
P54	Josie Herrold	University of Kansas	Pharm Chem
P56	Maryann Melendrez Cuadros	University of Kansas	Pharm Chem
P58	<u>Austin Petfalski</u>	Iowa State University	Pharm Chem
P60	<u>Colin Silva</u>	University of Kansas	Pharm Chem

### P1\_Synthesis and Study of a Series of Di-Aza Lanthanide Crown Ether Complexes

Aubrey G. Brown, <sup>1,2</sup> Grant A. Arehart, <sup>1</sup> Alexander C. Ervin, <sup>1</sup> and James D. Blakemore <sup>1</sup> Department of Chemistry, University of Kansas, Lawrence, KS <sup>2</sup> Department of Chemistry, Carthage College, Kenosha, WI

Lanthanides tend to be found in the +III oxidation state. Accessing lower valent forms could have applications in separations and a variety of technologies, but development of strategies to access more exotic oxidation states has not received the attention it deserves. In the work described on this poster, we hypothesized that coordinating lanthanide metals within a crown ether ligand would make reduced forms more accessible. Therefore, a series of di-aza crown lanthanide complexes was synthesized in order to understand the properties of such species. Prior to the synthesis of the complexes, lanthanide (La, Sm, Eu, Tm, Yb) triflate salts (Ln(OTf)<sub>3</sub>) were dried. After drying, lanthanide salts were dissolved in THF along with the crown ligand (LDAB), resulting in formation of the desired lanthanide complexes. To confirm the presence of the newly synthesized complexes, <sup>1</sup>H and <sup>19</sup>F NMR spectra were collected. A variety of characterization methods were used to study the isolated complexes, including cyclic voltammetry, UV-visible, infrared, and Raman spectroscopy, as well as single-crystal X-ray diffraction analysis. Findings from these experiments demonstrate the phenomenon known as the lanthanide contraction: as more protons are added to the lanthanide's nucleus, the poor shielding effect of the 4f electrons causes valence electrons to be pulled closer to the nucleus, resulting in effectively smaller atomic radii. Future experiments will prioritize the reduction of Ln(OTf)<sub>3</sub> using Ln<sup>0</sup>. Following this reduction, similar experiments will be conducted to compare differences between Ln<sup>III</sup> and Ln<sup>III</sup> complexes.

### P2\_Optimization of Parameters for Locally and Remotely Evoked Dopamine Release in Adult Zebrafish Brain

Ashleigh N. Caldwell, 1,2 Dineesha Chandrasiri, 1 and Michael Johnson 1

Dopamine is a vital neurotransmitter produced in brain regions such as the Substantia Nigra and Ventral Tegmental areas where it plays a key role in modulating NMDA receptor function. By modulating NMDA receptors, dopamine also plays a role in establishing Long Term Potentiation (LTP) – the cellular mechanism behind learning and memory. Parkinson's Disease is characterized by the degeneration of dopamine producing neurons, leading to reduced dopamine levels and impaired motor control amongst other symptoms. For this study, the model organism used is Zebrafish (Danio rerio) seeing as their brain contains about 10 million neurons as well as evolutionarily conserved neuronal pathways similar to those in humans. Their Dopaminergic system includes an ascending pathway resembling that of the Mesolimbic and Mesocortical circuit in the human brain. By using Fast Scan Cyclic Voltammetry (FSCV) to stimulate dopamine release, the interaction of dopamine and LTP can be further characterized. This project aims to optimize the parameters (current, frequency, and pulse rate) associated with stimulating dopamine release in order to maximize the efficiency and accuracy of FSCV used in this setting. Drug studies using Vanoxerine (GBR 12909) were also carried out to confirm dopamine as the molecule being observed.

<sup>&</sup>lt;sup>1</sup> Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup> Department of Chemistry, Murray State University, Murray, KY

### P3\_Heptafulvalene-like Dianions of Electrochromic 6,6'-Biazulenes

Raina Fair, Stephanie N. Pham, Mikhail V. Barybin Department of Chemistry, University of Kansas, Lawrence, KS

Azulene is a deep blue, non-benzenoid constitutional isomer of naphthalene. The intrinsic dipole moment of azulene arises from the intramolecular charge transfer involving its edge-sharing 5- and 7membered carbon rings. Due to its unique physicochemical characteristics, the azulenic scaffold constitutes an attractive building block in the design of advanced materials for applications in organic molecular electronics and optoelectronics. Our research group has recently demonstrated that the 6.6'biazulenic motif undergoes a one-step, 2-electron electrochemical reduction in CH<sub>2</sub>Cl<sub>2</sub>/nBu<sub>4</sub>NPF<sub>6</sub> with the half-wave potential (E<sub>1/2</sub>) being quantitatively tunable though functionalization along its molecular axis. In contrast, chemical reduction of such 6,6-biazulenes with decamethylcobaltocene occurs in two distinct 1-electron steps and leads to marked electrochromism associated with the formation of the biazulenic radical anions and dianions. The dianionic species is postulated to have a closed-shell, cycloheptafulvalene-like structure. In this project, we documented electrochemical reduction profiles of several linearly functionalized 6,6'-biazulenes in CH<sub>3</sub>CN/<sup>n</sup>Bu<sub>4</sub>NPF<sub>6</sub> media, which consistently showed less negative  $E_{1/2}$  values (i.e., easier reduction) compared to the corresponding  $E_{1/2}$  characteristics in CH<sub>2</sub>Cl<sub>2</sub>/nBu<sub>4</sub>NPF<sub>6</sub> solutions. The <sup>1</sup>H NMR analyses confirmed the diamagnetic nature of the thermally stable (but highly air- and moisture-sensitive) decamethylcobaltocenium salts of the 1.1'.3.3'tetraethoxycarbonyl-6,6'-biazulene dianion as well as the 2,2-diisocyano- and 2,2'-methylthioderivatives thereof.

### P4\_Building a Diagnostic for Stroke Using a Modular Microfluidic System

<u>Ellison Gee,</u><sup>1,2</sup> Sheila M. Barros,<sup>2,3</sup> Favour Nwachukwu,<sup>2,3</sup> Pubudu Premarathne,<sup>2,3</sup> Malgorzata A. Witek,<sup>2,3,4,5</sup> Alison E. Baird,<sup>6</sup> Steven A. Soper<sup>1,2,3,4,5,7</sup>

<sup>1</sup>Department of Mechanical Engineering, The University of Kansas, Lawrence, KS, <sup>2</sup>Center of BioModular Multi-scale Systems for Precision Medicine, The University of Kansas, Lawrence, KS, <sup>3</sup>Department of Chemistry, The University of Kansas, Lawrence, KS, <sup>4</sup>Department of Cancer Biology, The University of Kansas Medical Center, Cancer Center, Kansas City, KS, <sup>5</sup>Kansas Institute for Precision Medicine, University of Kansas Medical Center, Kansas City, KS, <sup>6</sup>SUNY Downstate Medical Center, Brooklyn, NY, <sup>7</sup>Bioengineering Program, The University of Kansas, Lawrence.

A device that can distinguish between stroke subtypes (ischemic and hemorrhagic) within the ideal time window from symptom onset (<4.5 h) with high accuracy and faster than current techniques (CT or MRI imaging) is an unresolved diagnostic challenge. We are developing an integrated system to meet this challenge, which consists of several functional modules. This work focused on a single module: Solid Phase Reversible Immobilization (SPRI) microfluidic chip; the goal of the SPRI chip is to purify RNA from extracellular vesicles (EVs). Fabrication of the SPRI chip includes hot embossing micropillar-populated fluidic channels into a COC thermoplastic. UVO<sub>3</sub> treatment of the chips increased their wettability and added oxygen groups to the micropillars, which aids in the immobilization of RNA. EV's are harvested from HL60 cells and precipitated to increase their purity and concentration. The EVs are lysed and their cargo along with multiple reagents, are pushed through the SPRI chip at varying flowrates for immobilization, purification, and release of the purified RNA. Multiple trials of the SPRI chip, as well as a control using a commercial kit, were performed. We show efficient purification of RNA secured from bloodbased stroke biomarkers (i.e., CD-15 expressing EVs). The typical mass of total RNA eluted from the chip is ~100 ng from samples with 9.12•10<sup>11</sup> EVs/ml. By refining this module, we advance the platform's capabilities and give a starting point for future assays that will use the purified RNA for stroke diagnosis using specifically mRNA expression profiles.

### P5\_Exopeptidase Digestion of Peptides in a Microfluidic Device

<u>Austin Groth</u>, <sup>1,2</sup> Pramodi Vithanage, <sup>1</sup> Steven Soper <sup>1</sup>

Protein function is correlated to its structure, which determines its role in disease and other phenotypes. Thus, the knowledge of a disease-associated protein's structure can help to identify treatments with higher efficiency for that disease. However, current peptide sequencing techniques like Edman degradation and mass spectrometry are limited in their sequencing applicability due to their high cost, relative inability to identify post-translational modifications (PTMs), and limitations on sample size and type. Thus, there is a need to push for cheaper, more efficient solutions for protein sequencing. Solidstate and biological nanopores can bridge the gap associated with current protein sequencing techniques by providing high sensitivity even at the single-molecule level, ability to detect PTMs, and highly optimized usage of resources. Carboxypeptidase Y (CPY) is an exopeptidase with broad substrate specificity that cleaves single amino acids from peptides. CPY was immobilized onto cyclic olefin copolymer (COC) microchip by EDC/NHS coupling chemistry to perform solid-phase digestion. Microfluidic digestion offers a simplified, high-throughput format for optimizing reaction conditions prior to integration into nanoporebased sequencing platforms. Solution and solid-phase digestion experiments were conducted to evaluate the efficiency of CPY for digesting model peptides. The digestion products were analyzed using reversephase liquid chromatography mass spectrometry (LC-MS). Results from the digestion of met-enkephalin peptide indicates that immobilized CPY retains enzymatic functionality and is capable of solid-phase digestion. Solid-phase digestion offers several benefits including the elimination of enzyme autodigestion and thus, the ability to be directly integrated to nanopores for identifying and detecting single amino acids.

#### P6\_Phagocytosis Regulation of Disease-Associated Microglia and Astrocytes

Autumn R. Harris, 1,2 Jack M. Petersen, 1 Matthew C. Zupan, 1 Meredith D. Hartley 1

Alzheimer's disease is a neurodegenerative disease that affects memory and cognitive function as the disease progresses over time. While other researchers have found treatments to manage Alzheimer's disease, there is currently no cure. It has been found that a protein called amyloid-ß that aggregates into amyloid-ß plaque could possibly be a cause of Alzheimer's disease. The amyloid-ß plaque binds to neurons which leads to a disruption within the brain. This disruption is thought to be associated with Alzheimer's Disease. The two main cells that we focused on were microglia and astrocytes, because of their ability to phagocytose cellular debris. Both glial cells can phagocytose amyloid-ß plaque through phagocytosis or cellular eating. Using various treatment times we want to observe how much each cell phagocytosed. Our experimental treatment involved using primary cells from rat pup brains and treating them with A-beta, myelin, and fluorescent beads. The cells were also treated with carnosine which is a naturally occurring dipeptide that is shown to have beneficial effects in reducing the toxic response of cells exposed to A-Beta. We believe that carnosine will have a therapeutic effect by increasing the rate of phagocytosis of cellular debris in Alzheimer's Disease.

<sup>&</sup>lt;sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup>Department of Chemistry, Midwestern State University, Wichita Falls, TX

<sup>&</sup>lt;sup>1</sup> Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup> Department of Chemistry, Langston University, Langston, OK

### P7\_Baseline Profiling of an Accessible Human Triculture Model for Neuroinflammation

Patryk Hupert, <sup>1, 2</sup> Jay Sibbitts, <sup>1, 3</sup> Andrea Graziani, <sup>7</sup> Giuseppe Caruso, <sup>6</sup> Susan M. Lunte, <sup>1, 4, 5</sup> <sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS, <sup>2</sup>Department of Molecular Biosciences, University of Kansas, Lawrence, KS, <sup>3</sup>Department of Chemistry, Truman State University, Kirksville, MO, <sup>4</sup>Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS, <sup>5</sup>Adams Institute for Bioanalytical Chemistry, University of Kansas, Lawrence, KS, <sup>6</sup> Department of Pharmacology, Saint Camillus International University of Health Sciences, Rome, Italy, <sup>7</sup>Department of Molecular Biosciences, Saint Camillus International University of Health Sciences, Rome, Italy

Alzheimer's Disease (AD) is a neurodegenerative disorder characterized by the deterioration and eventual death of central nervous system cells. Amyloid-beta plaques are a hallmark of AD; however, repeated failures of therapies targeting these plagues have cast doubt on their central role in disease causation, and Alzheimer's remains incurable. However, growing evidence suggests neuroinflammation is a key factor in understanding neurodegenerative pathologies. Therefore, our research aims to develop tools for modeling and investigating neuroinflammation. Traditional mono-culture models inadequately represent neuroinflammation due to their lack of essential cell-to-cell communication. Existing mixed culture models better reflect biological complexity but often rely on specialized techniques and costly materials that limit accessibility to researchers. To overcome these limitations, our system is made with only commercially available cells and materials, incorporating three cell types that are central to neuroinflammation, microglia (HMC3), astrocytes (HA), and neurons (SH5Y-SY). Imaging and cell counting analyses of the triculture system show that the cells are viable. A method using high performance liquid chromatography (HPLC) with diode array detection was developed to measure intracellular energy metabolites including adenine nucleotides, redox cofactors, and related purine derivatives. RNA sequencing is used as a method to characterize transcriptomic variations at basal conditions between the tri-culture and monoculture, with principal component analysis to visualize sample level variance and differential expression analyses to confirm experimental model driven variance. These metabolomic and transcriptomic analyses will provide insight to help determine whether this approach warrants further investigation.

#### P8 Affinity Characterization of Novel Polyclonal Antibodies for an Ovarian Cancer Biomarker

Spencer Moffitt, 1,2 Anubhuti Srivastava,1 and Rebecca J. Whelan1

<sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS

<sup>2</sup>Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH

CA125, a peptide epitope on the MUC16 protein, is the gold standard biomarker for ovarian cancer. M11 and OC125 are the two antibodies currently used to detect CA125 in a sandwich enzyme-linked immunosorbent assay (ELISA). Previous studies have shown that these antibodies do not bind uniformly to the tandem repeat region of MUC16, where CA125 is found, leading to false negatives. The objective of this project was to characterize the affinity of novel antibodies for individual tandem repeats of MUC16. Novel antibodies were generated against three well conserved peptide sequences in the tandem repeats. The antibodies were generated in two rabbits to confirm the reproducibility of the antibodies. The binding interaction of each tandem repeat with the antibodies was measured using indirect ELISA and Western Blot. The binding pattern was generally in agreement between the antibodies generated from the two rabbits. Antibody 1 was found by ELISA to bind to 9 of the 16 repeats tested, while Western Blot found it to bind to 12 of the 16 repeats. Antibody 2 was found by both ELISA and Western Blot to bind to all of the repeats tested. Antibody 3 was found by ELISA to bind to 12 of the 16 repeats tested, while Western Blot found it to bind to 15 of the 16 repeats. Overall, antibody 2 bound more uniformly to the tandem repeat region than OC125. Future work will focus on utilizing antibody 2 in detecting fully intact MUC16.

# P9\_Preparation and Polymerization of Cyclic Ketones for Rearrangement Based Functionalization

Jamie E. Neumann, 1,2 Peace Adelowokan, 1 Aaron J. Teator 1

Medium sized (7-8 membered) functionalized cyclic ketones are very efficient monomers due to their ability to undergo ring opening metathesis polymerization (ROMP), driven by their inherent ring strain. ROMP allows for controlled polymerization of cyclic unsaturated compounds, while the ketone allows for post polymer functionalization. This cyclic ketone monomer was prepared from cyclooctadiene through a 3-step synthesis involving an epoxidation, reduction, and oxidation reaction. This was polymerized through ROMP using a Grubbs-type catalyst to yield a polyketone. Three different molecular weights of the polymer were synthesized and characterized to ensure the chemistry stayed consistent through different degrees of polymerization. Post-polymerization functionalization was performed where the polyketone was converted to a polyoxime through an oximation reaction. Products were characterized using <sup>1</sup>H and <sup>13</sup>C NMR, gel permeation chromatography (GPC), infrared (IR) spectroscopy, thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC). GPC analysis suggests that the polymerization stayed controlled and there were no unwanted side reactions that occurred during the oximation step. A Beckmann rearrangement was attempted to convert the polyoxime to a polyamide. inserting nitrogen into the backbone of the polymer. Preliminary IR spectroscopy data indicates the possible formation of a nitrilium ion; however, solubility issues have limited full characterization of this unknown product. Efforts to optimize the reaction conditions are in progress to allow for further characterization and promote full conversion to the amide. This work contributes to the development of controlled polymers with tunable backbones through post polymer functionalization, offering new strategies for designing materials with specific properties.

# P10\_Variation in Reaction Rates of an Oxo-bridged Manganese-Cerium Complex using Substituted Phenols

Daisy G. Orozco, 1,2 Anagha Puthiyadath, 1 and Timothy A. Jackson 1

<sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS, <sup>2</sup>Department of Natural Health and Mathematical Sciences, MidAmerica Nazarene University, Olathe, KS

Cerium Ammonium Nitrate (CAN) is a strong oxidant commonly used in catalytic and stoichiometric processes that require the conversion of low- or mid-valent transition metals to high-valent complexes. For example, CAN is used as an oxidant in transition-metal-catalyzed water oxidation. CAN has a strong oxidizing power due to the high reduction potential of the Ce<sup>IV</sup>/Ce<sup>III</sup> couple. CAN is also a strong Lewis acid which will produce many products with one of them being metal-oxygen-cerium adducts. A study in the lab found that reacting [Mn<sup>III</sup>(OH)(PaPy<sub>2</sub>Q)]<sup>+</sup> with one equivalent of CAN did not oxidize the Mn<sup>III</sup> center as expected. Instead, Ce<sup>IV</sup> acted as a Lewis acid to convert the Mn<sup>III</sup>-OH complex into an Mn<sup>III</sup>-O-Ce<sup>IV</sup> complex. The reactivity of the Mn<sup>III</sup>-O-Ce<sup>IV</sup> complex using 4-R-2,6-ditert-butylphenols (4-R-2,6-DTBP), where R denotes the substituents (R= OMe, Me, tBu and CI). Exploring the reaction using these various para-substituted phenols will allow us to observe how the changes in the thermodynamic properties of the substrate correlate with the reactivity of the Mn<sup>III</sup>-O-Ce<sup>IV</sup> complex. These results can be compared to a prior study of the reaction of 4-R-2,6-DTBP with the analogous Mn<sup>III</sup>-OH complex.

<sup>&</sup>lt;sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup>Department of Chemistry, University of Wisconsin Eau Claire, Eau Claire, WI

### P11\_Dual Catalytic System for Decarboxylative Aromatization of Saturated Cyclic Carboxylic Acids

<u>Jermiah A. Polk</u>, <sup>1,2</sup> Colin W. Waller, <sup>1</sup> Jon A. Tunge <sup>1</sup>

<sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS, <sup>2</sup> Department of Chemistry and Biochemistry, Abilene Christian University, Abilene, TX

Catalytic dehydrogenation of saturated feedstocks is an attractive strategy for the synthesis of valuable aromatic compounds. Whereas former methods for catalytic dehydrogenation typically rely on a hydrogen atom transfer (HAT) from a hydridic C-H bond to initiate dehydrogenation, we report a cobalt/quinone dual photocatalytic system for the decarboxylative aromatization of saturated cyclic carboxylic acids. Unlike prior strategies, which demonstrate strict regioselectivity controlled by electronic effects, the proposed catalytic system proceeds via radical decarboxylation of readily available carboxylic acids to promote dehydrogenation and subsequent aromatization under mild conditions and evades the need for hydridic C-H bond activation. To optimize reactivity, we screened a series of halide-substituted quinone derivatives for their capacity to perform single electron transfer (SET) and have observed that the oxidative SET appears to be best facilitated by 2chloroanthraquinone against 2-bromoanthraquinone and the unsubstituted anthraquinone. We also tested the reaction scope by subjecting a series of functionally diverse substrates to the reaction conditions. In investigating this decarboxylative approach, we have shown its increased selectivity, demonstrating its usefulness in late-stage functionalization.

# P12\_Fabrication of Gold Nanotriangle Arrays and LSPR Characterization for Biosensing Applications

Keimarya Rivera, 1,2 Nimodi Uduwela, 1 Chris Johnson, 1 Cindy L. Berrie 1

Metallic nanostructure arrays have a wide range of applications in industry and medicine through the utilization of enzymatic cascades for synthesis and biosensing. However, current strategies require complex, expensive equipment, lack recyclability and recovery of nanostructured platforms, and cannot get down to optimal sizes for these applications. This study explores the design of a robust fabrication of highly ordered gold nanotriangles on a glass substrate utilizing nanosphere lithography (NSL) and thermal evaporation. The mask for NSL was formed via the air-water interface method which utilizes the self-assembly of hexagonally packed polystyrene nanospheres. The deposition of gold through the mask via thermal evaporation followed by the removal of spheres formed a uniform array of gold nanotriangles. Gold nanotriangle sizes and spacing were altered by the utilization of different sized nanospheres. Sample characterization was done with Confocal microscopy for packing density of larger sphere sizes, Atomic Force Microscopy (AFM) for detailed heights and widths of nanotriangle features, and UV-Vis-NIR for localized surface plasmon resonance (LSPR) of the structures. This resulting method utilizes the Marangoni effect (movement from high to low surface tension), a 0.1 mM SDS in the sub phase, and a < 45° drying angle to achieve a homogeneous monolayer of 900 nm diameter polystyrene spheres with well-defined (240.00 ± 6.08 nm width) triangle arrays. Preliminary experiments were carried out to test their LSPR peaks and suitability as biosensors. Further work aims to optimize the conditions for monolayers made by 100 nm spheres by increasing the concentration of SDS.

<sup>&</sup>lt;sup>1</sup> Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup> Department of Chemistry, Oglethorpe University, Atlanta, GA

### P13\_Probing the Reaction of the Hydrated Electron and Zn2+

Landon E. Scott, 1,2 Wilberth A. Narvaez, David M. Bartels, and Ward. H Thompson David M. Bartels, And Ward. H Thompson

Direct ionization of water molecules can generate a highly reactive species known as the hydrated electron  $(e_{aq}^-)$ , one of nature's strongest reducing agents. Understanding the behavior of  $e_{aq}^-$  is critical for applications ranging from nuclear reactor chemistry to radiation therapy. Experimental studies have found that its reactions with a wide variety of organic solutes all exhibit activation energies  $(E_a)$  within a range of 6 kJ/mol despite a wide range of reaction free energies  $(\Delta G_{rxn})$ . This behavior is inconsistent with Marcus theory, the standard description of electron transfer reactions, which predicts that more exergonic (endergonic) reactions should exhibit lower (higher) activation. To explore this unusual behavior for hydrated electron reactions, including beyond organic reactants, we are examining the reaction:  $e_{aq}^- + Zn^{2+}(aq) \rightarrow Zn^+(aq)$ , which involves a transition metal with a closed shell (3d¹o) electron configuration and a measured activation energy of  $E_a^- = 37.0$  kJ/mol, significantly higher than that observed with organic reactants. Using ab initio molecular dynamics (AIMD) simulations, this investigation aims to uncover new insights into the solvation environment of the hydrated electron and its unique reactivity with both organic and inorganic solutes.

### P14\_Differential mRNA Profiling in an In Vitro Stroke Model

Brandon T. Sikes, 1,2 Nwachukwu C. Favour 1,3, and Steven A. Soper 1,3,4,5

<sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS, <sup>2</sup>Washington University in St. Louis, St. Louis, MO, <sup>3</sup>Center of BioModular Multiscale Systems for Precision Medicine, Lawrence, KS, <sup>4</sup>Department of Mechanical Engineering, University of Kansas, Lawrence, KS, <sup>5</sup>Bioengineering Program, University of Kansas, Lawrence, KS.

Stroke remains a major U.S. public health issue, with a new case every 40 seconds and a death every 3 minutes. Globally, stroke generates over 160 million Disability Adjusted Life Years lost and an economic burden of \$56.2 billion/year. Timely and accurate diagnoses are essential, yet CT and MRI imaging methods introduce accessibility issues such as cost and reduced sensitivity during the critical time of early onset of stroke. Diagnostic approaches are urgently needed to guide early decision-making and treatment, particularly in pre-hospital settings. These are especially important, given FDA-approved therapy with tissue plasminogen activator is available for ischemic stroke within effective therapeutic window of <4.5 h and is contraindicated in hemorrhagic stroke. This study sought to generate an in vitro cellular model to simulate stroke subtypes and evaluate distinct mRNA gene expression profiles to validate a selected gene panel for diagnosis of both ischemic and hemorrhagic stroke. HL60 cell line was used because these cells exhibit high neutrophil-like expression of CD15 antigen aligning with the target immune cell subtype for endpoint diagnostic applications. Ischemic stroke was modeled by stimulating cells with lipopolysaccharide, while hemin was used to simulate hemorrhagic stroke. After stimulation, total RNA was extracted for downstream analysis. Reverse transcription quantitative real-time PCR (RTqPCR) uncovered differential gene expression patterns between the two stroke-mimicking conditions. These findings support the application of this system as a platform for investigating molecular markers of stroke subtypes and will contribute to developing a microfluidic-based diagnostic capable of distinguishing these molecular markers in pre-hospital setting.

<sup>&</sup>lt;sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup>Department of Chemistry, Baker University, Baldwin, KS

<sup>&</sup>lt;sup>3</sup>Radiation Laboratory, University of Notre Dame, Notre Dame, IN

# P15\_Development of a Liquid Biopsy Method for Early Detection of Ovarian Cancer Using Extracellular Vesicle-Derived Fallopian Tube Biomarkers

Lily S. Tackett, Bhagya Samarakoon, Rebecca J. Whelan

Department of Chemistry, University of Kansas, Lawrence, KS

High-grade serous ovarian carcinoma (HGSOC) is the deadliest ovarian cancer subtype, primarily due to late-stage diagnosis and the lack of sensitive biomarkers for early detection. Emerging evidence suggests HGSOC originates in the fallopian tubes, where extracellular vesicles (EVs) released by epithelial cells carry potential biomarkers. Among these, integrin beta-3 (ITGB3) is a key surface protein elevated on HGSOC-positive EVs. The s10yh2 aptamer binds ITGB3 and shows promise for EV-based detection, but nonspecific binding to serum albumins limits its accuracy in clinically relevant conditions. We are developing an assay to reduce nonspecific binding by immobilizing EVs via capture antibodies targeting common EV surface markers. ITGB3 detection was achieved by measuring fluorescence intensity and anisotropy upon binding of Texas Red-labeled s10yh2. EVs were isolated from fallopian tube cell culture media (CCM) and characterized by nanoparticle tracking analysis (NTA) and BCA protein assay, confirming a size range of 100-300 nm, a concentration of 1x10<sup>12</sup> EVs/mL, and a protein concentration of 1900 ± 100 µg/mL. Immunoblot confirmed the presence of the EV surface marker Ep-CAM. We found optimal capture antibody concentration to be 1 µg/mL for anti-EpCAM, with a 15minute incubation each. Flow cytometry-based detection of ITGB3 and additional assay optimizations are underway. Future work will apply the assay to human serum, ascites, and EVs from healthy cells as well as from early- and late-stage HGSOC cells to evaluate diagnostic potential.

#### P16\_Synthesis and characterization of site-differentiated heterometallic Ni-Zn assemblies

William Viator, 1,2 Fernando Gonzalez, 1 Manar Shoshani 1

An intriguing area of organometallic research is based on the conversion of raw and abundant feedstock materials into value-added products. Such transformations have proven difficult due to the primarily inert bonds of these substrates; however, nature has shown numerous examples of enzymes being able to perform challenging conversions, such as CO<sub>2</sub> reduction through the Ni-Fe-CODH active site, which utilizes Ni alongside a Lewis-acidic Fe center. Inspired by nature, well-defined heterometallic complexes have been explored in homogeneous catalysis with the goal of fine-tuning catalyst designs to access challenging molecular transformations. Previous work done in the Shoshani lab has involved the design of systems to access well-defined heterometallic species, such as a Ni-Mg bisphosphine complex, which is capable of performing challenging reductive chemistry. To continue to explore the role of Lewis-acidic cations, synthetic routes to incorporate Zn into the Ni-containing scaffold were explored. The synthesis, characterization, and reactivity of a novel and well-defined Ni-Zn<sub>2</sub> complex will be discussed. Studies to understand the synthetic pathway, catalytic activity, and reduction potential will also be discussed.

<sup>&</sup>lt;sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup>Department of Chemistry and Physics, Louisiana Tech University, Ruston, LA

### P17\_Estrogen Depletion Effects on Lipid Homeostasis and Myelination

Karissa Wilson, 1,2 Esther Holt1, Matthew C. Zupan1, Meredith D. Hartley1

The myelin sheath is a lipid-rich substance that coats the axons of neuronal cells. It allows for quick and efficient travel of electrical signals throughout the central nervous system. However, when this sheath degrades—or demyelinates—the speed at which signals can transmit decreases significantly, and in some cases the travel is inhibited altogether. Multiple sclerosis, or MS, is the most common demyelinating disease in the US, with nearly one million Americans having been diagnosed, and it continues to become more prevalent with every passing year. Although anyone can develop the disease, women are four times more likely to get MS compared to men. Females diagnosed with multiple sclerosis, or MS, tend to see the least amount of disease progression during pregnancy, and the greatest amount during menopause, suggesting a potential link between estrogen production and remyelination. To further investigate this relationship, we used an inducible conditional knockout mouse model where demyelination can be induced via tamoxifen injections. Ovariectomies were performed on female mice to block estrogen production. The mice were perfused and histology and immunofluorescence experiments were performed on the brain to determine the effects of estrogen depletion on myelination.

### P18\_The Impact of Weather Disruptions on Public Transit Performance in Kansas City

Nathan Binshtok<sup>1,2</sup> and Joel Mendez<sup>1</sup>

<sup>1</sup>University of Kansas School of Public Affairs and Administration

The increasing frequency and severity of extreme weather events pose a significant challenge to public transportation infrastructure. Severe weather has demonstrated effects on transit infrastructure, operations, and reliability; effects which trickle down to customer behavior and individual choices. In response, transportation agencies have adopted emergency management, operational adaptability, and continuity planning approaches. The efficacy of these practices can be assessed, in part, by examining customer complaints. Previous studies have examined customer complaints as proxies for service disruptions and found impacts on transit ridership. In order to connect the understood influence of weather events on public transit and the impact of customer complaints, this study explores the intersection of severe weather, transit operations, and ridership experience using customer complaints as a diagnostic tool. Importantly, not all riders are affected equally. Socially vulnerable groups experience a disparity in the hardship caused by infrastructure service disruptions, particularly as a result of weather perturbations. Ensuring equitable service during and after extreme weather events is essential to maintaining trust and accessibility in public transit systems with respect to perceived service quality. Through understanding the implications of complaint data and other service metrics, transit agencies can take strides towards more equitable, resilient, and reliable public transportation.

<sup>&</sup>lt;sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup>Department of Chemistry, Bethel College, North Newton, KS

<sup>&</sup>lt;sup>2</sup>University of Kansas Department of Economics

### P19\_Lawrence Synthetic Water Distribution Network

Joshua Burns, 1,2 Hannah Gideon, 2,3 Benjamin Lofland, 2 Justin Hutchison, 2 Edward Peltier 2

This work proposes methodological improvements for generating synthetic water distribution networks in EPANET, focusing on adaptable solutions for rural and small town systems where infrastructure data is limited. While existing tools map pipes along road networks, key challenges remain realistically representing variable water sources (wells, rivers, tanks) and elevation driven hydraulic behavior. This paper suggests targeted strategies to address these gaps, including: (1) rule-based source placement tied to local terrain and demand clusters, (2) elevation aware zoning to simulate pressure differences in hilly or flat regions, and (3) demand allocation methods that reflect rural settlement patterns. By decoupling deterministic pipe routing (road-following) from flexible source and elevation logic, the approach balances structural realism with scenario testing versatility. The ideas aim to guide future coding efforts, helping communities model their systems more accurately even with incomplete data. Practical applications include preliminary infrastructure planning, resilience testing, and prioritizing field data collection. Future work could formalize these strategies into open source tools or integrate them with crowd sourced elevation datasets.

### P20\_Connecting the Community Capitals to Housing

Ryan Corrigan, 1,2 Yongwang Ren,2 Zander Seth,2 Jacob Wendland,2 and Jason Bergtold2 Department of Political Science, University of Kansas, Lawrence, KS2 Department of Agricultural Economics, Kansas State University, Manhattan, KS

Housing is a prerequisite for health, well-being, and economic security. Without it, the ability to invest in the future may become compromised. Housing insecurity – defined as the uncertain access to stable, safe, and affordable housing – is operationalized as the percentage of households paying more than 30% of their household income on housing costs. As a result, housing outcomes are influenced by interactions among community capitals, which encompass the assets that support a community, ranging from the social capital that connects people to the built capital that sustains them. Thus, the purpose of this study is to investigate the influence of community capitals on housing insecurity at a county level across Kansas. First, we create a dataset of indicators for the seven community capitals across the counties of Kansas from 2017 to 2022. Then, we develop community capital indices using factor analysis to reduce the dimensionality for each community capital. Finally, we estimate regressions to understand the relationship between the community capitals and housing insecurity. We expect counties with low levels of housing insecurity to exhibit high levels of built, social, and human capital. On the other hand, counties with high levels of housing insecurity, we expect to exhibit low levels of built, social, and human capital. Our findings identify the community assets that drive housing security, highlighting housing as a vital foundation of resilient communities.

<sup>&</sup>lt;sup>1</sup>University of Kansas Mechanical Engineering

<sup>&</sup>lt;sup>2</sup>University of Kansas Civil, Environmental, and Architectural Engineering Department

<sup>&</sup>lt;sup>3</sup>Fort Hays State University Department of Geosciences,

# P21\_Quantifying Chloramine Residuals and Pathogen Presence in Lawrence's Drinking Water Distribution System

Hannah Gideon,<sup>1,4</sup> Joshua Burns,<sup>2,4</sup> Benjamin Lofland,<sup>3</sup> Justin Hutchison,<sup>3</sup> Edward Peltier<sup>3</sup>

Chlorinated water distribution systems are widely utilized across the United States due to their effective disinfection capabilities. While free chlorine serves as a primary disinfectant, it decays rapidly within distribution systems as temperature increases. Ammonia is added to increase disinfectant stability, reacting with free chlorine to form a secondary, slow-decaying disinfectant known as monochloramine. Limited continuous testing locations present challenges for evaluating variations in water quality throughout distribution systems across the United States. This research examines the concentrations of total chlorine, monochloramine, and free ammonia at several sites within the Lawrence, Kansas, Water Distribution System. Results indicated a consistent, stable presence of all three compounds across most sites, suggesting effective maintenance of disinfectants. One site indicated lower concentrations of disinfectants, implying nearby water quality degradation. Findings demonstrate that continuous monitoring of water distribution systems is vital to the resilience of water safety within communities. Future implementation of synthetic water quality modeling tools that utilize collected data can significantly enhance public health resilience by reducing the risk of waterborne illnesses across the United States.

### P22\_Understanding the Removal of Bacteria from our Wastewater to Safeguard our community.

Matthew Goodman, 1,2 Dev Hiripitiyage, 2 Belinda Sturm<sup>2</sup>

<sup>1</sup>University of Kansas Chemical and Petroleum Engineering Department <sup>2</sup>University of Kansas Civil, Environmental and Architectural Engineering Department.

Wastewater is a critical but often overlooked part of our community's infrastructure. It provides clean water for our community's, farmers, and industry. It is crucial that the processes of filtration for this remain effective against pathogenic bacteria. Our research focuses on the protozoa's biological process of consuming and removing pathogenic bacteria and understanding the rate of the process. This understanding will allow us to treat our wastewater more effectively and provide a more resilient and faster wastewater filtration system. We worked on this experiment by quantifying the rate of removal of bacteria in comparison of the number of stalked ciliates. This was done through a dilution of fluorescent E. Coli and a sample of synthetic wastewater. Through colony counts and comparison between a negative control, our hypothesis is that the stalked ciliates actively graze upon the E. Coli and provide a significant decrease in their concentration. This is important as a greater increase of removal of E. Coli leads to a faster filtration rate leading to a greater capacity of wastewater facilities and a more effective filtration.

<sup>&</sup>lt;sup>1</sup>Fort Hays State University Department of Geosciences

<sup>&</sup>lt;sup>2</sup>University of Kansas Mechanical Engineering,

<sup>&</sup>lt;sup>3</sup>University of Kansas Civil, Environmental, and Architectural Engineering

### P23\_Race Against the Clock: Smart Crew Allocation Strategies for Rapid Urban Recovery

Emily Greer, Rahul Madbhavi, Balasubramaniam Natarajan

Electrical and Computer Engineering, Kansas State University

Timely restoration of critical infrastructure after natural disasters is crucial to preventing cascading system failures and limiting socioeconomic impacts. The growing frequency and intensity of natural disasters have severely disrupted interdependent urban infrastructure systems, especially power distribution networks. Traditional restoration approaches prioritize minimizing outage duration for the largest number of customers, often overlooking broader community-level needs and contributing to inequities in service recovery. Existing methods focus on crew dispatch and repair sequencing, but many fail to account for population density, crew capabilities, and complex routing logistics under certain constraints. Our approach to this is a mixed-integer linear programming (MILP) framework that optimizes crew allocation, while factoring in travel and repair times, population weight, and minimizing the makespan. We validated our methodology through a co-simulation framework that integrates damage modeling, crew dispatch, and network restoration. This significantly reduces overall restoration time, improves fairness by minimizing delays in highly populated areas, and demonstrates scalability in cases with uneven crew-to-location ratios.

# P24\_Faster Settling, Safer Cities: Enhancing Sludge Settleability to Boost Clarifier Flow Capacity

Monique Haynie, 1,2 Megan Wittman, 1 Belinda Sturm 1

<sup>1</sup>University of Kansas Civil, Environmental, and Architectural Engineering Department <sup>2</sup>University of Kansas Chemical and Petroleum Engineering Department

Heavy rainfall creates hydraulic overloads at wastewater treatment plants (WWTPs) resulting in untreated sewage bypasses that discharge directly into natural water bodies. The secondary clarifier at WWTPs limits the flow throughput of the plant as the influent flow cannot be higher than the settling velocity of activated sludge. A pilot scale reactor was utilized to examine the impact of operational modifications on sludge settling velocity to boost secondary clarifier flow capacity, ultimately reducing bypass occurrences. Specifically, two operational metrics were evaluated at high and low extrema; 1. The anaerobic hydraulic residence time (HRT) needed for dense particle sludge formation in activated sludge basins, and 2, the organic loading rate (OLR) needed for floc-forming microorganisms to consume carbon. Sludge settling behavior was evaluated with batch testing methods to evaluate the intrinsic settling classes (ISC) and the settling velocity (vs). A longer anaerobic HRT of 120 minutes resulted in bigger, denser particles, confirmed with microscopy, sludge settling class determination, and a vs of 144 gal/day which is much greater than the pilot flow of 38 gal/day. Alternatively, the shorter anaerobic HRT of 20 minutes resulted in smaller and finer flocs, with 70% of the activated sludge being fines settling very slowly. The higher OLR condition had faster settling sludge than the lower OLR condition. This indicates that longer retention times and high carbon uptake rates promote granule formation which enhances both settleability and clarifier resiliency. For future work, these methods will be utilized in pilot clarifiers while simulating storm surges to study sludge behavior under elevated flow conditions. This work can help develop more durable wastewater treatment operations during severe weather conditions.

### P25\_Building Resilient Urban Food Systems through Place-Based Agricultural Strategies

David Hipp, 1,2 Shakil Kashem, Ph.D., AICP,2 Maria Binte Edrish2

<sup>1</sup>University of Illinois Department of Urban and Regional Planning

Place-based urban agriculture initiatives have the potential to increase resilience, build community, and make fresh food more accessible within cities. This study evaluates suitability for locally managed growing spaces across census tracts in both Kansas City, Kansas and Kansas City, Missouri, identifying areas most likely to benefit from urban agriculture. Tracts with high social vulnerability and low access to food stand to benefit the most from these initiatives. Suitability was assessed through a multi-criteria analysis incorporating slope, proximity to Toxic Release Inventory sites, flood susceptibility, soil type, and current land use. Using ArcGIS, these spatial factors were scored and compared to identify optimal locations for urban food production in the Kansas City area. The results from this study can be used to better understand Kansas City's suitability for urban agriculture and influence urban planning practices, leading to a more resilient urban food system.

### P26\_Enhancing Resilience Analysis with Daily Solar Clustering

King Nguyen, Demy Alexander, Visvakumar Aravinthan

Wichita State University Electrical and Computer Engineering Department

As renewable energy is more important, power systems face growing challenges in maintaining and resilience during disruption. Modeling resilience requires capturing low or no-generation events—especially for variable resources like wind and solar. While centralized wind and solar farms offer accessible data, distributed rooftop solar remains largely invisible to grid operators, making it difficult to assess its contribution during extreme events. Traditional seasonal grouping has been used to analyze and gather information to help in resilience studies, but this method is limited. At the same time, Wind generation is independent and highly time-dependent and sensitive to local weather conditions. As solar becomes a larger share of total generation, system volatility increases, and spatial-temporal variability becomes more critical. To address this, we propose a new method for grouping solar data based on daily patterns by comparing the behavior of each day. This approach improves the accuracy of groupings, captures weather-driven variability, and provides more meaningful inputs for resilience studies.

<sup>&</sup>lt;sup>2</sup>Kansas State University Department of Landscape Architecture and Regional & Community Planning

# P27\_Aridity Pathways of Communities under Similar Climate Classification: Implications for Summer Crop Production

Joseph Schauwecker, 1,2 Ikenna Onyekwelu, 2 Vaishali Sharda 2

As climate variability becomes more prevalent, developing agricultural resilience becomes critical to ensure yields are adequate for our future. This study explores long-tern trends in the aridity index (AI) and its impacts on summer crops: corn and sorghum in three counties with strong agricultural industries in western Kansas: Ford, Finney, and Scott counties. Despite sharing a similar Koppen-Geiger climate classification, we hypothesized that these communities do not experience similar aridity dynamics and impacts on summer crop outcomes. Using climate data from NASA POWER and PRISM, we computed potential evapotranspiration using the Hargreaves-Samani method and cumulative long-term rainfall for each county over the 1984- 2024 growing seasons. Additionally, Al trends in the three communities and their correlation with crop yield and silage production were assessed. Results revealed no strong longterm trends in aridity, but distinct impacts on crop response across the counties were observed. Al trends in Scott and Finney counties revealed strong symmetry and overlap in confidence intervals but showed asymmetric patterns in Ford County. Our results further showed that, in Ford County, growing season rainfall was the dominant factor influencing AI. In Scott County, both growing season rainfall and topsoil wetness were significant, while Finney County showed the most complex interactions, with solar radiation, relative humidity, growing season rainfall, and topsoil wetness having significant impacts. Overall, these results underscore the need for localized aridity assessments and communityspecific adaptation strategies, even within similarly classified climate zones.

### P28 Logging Atmospheric Conditions to benchmark in House Sensor

Aneesh Kaarthik Sivakumar, 1,2 and Garret Peterson<sup>2</sup>

<sup>1</sup>The Birla Institute of Technology and Science Department of Electrical and Electronics Engineering, <sup>2</sup>Kansas State University Department of Electrical and Computer Engineering Department

This research investigates the performance characteristics of a custom-built gas sensor by benchmarking it against the Bosch BME688, a metal-oxide semiconductor (MOS) gas sensor capable of detecting multiple volatile organic compounds (VOCs). The study aims to quantify the sensitivity and accuracy of the in-house sensor under controlled temperature and gas concentrations. The BME 688 was interfaced using an esp32 and evaluated over extended measurement intervals. Data analysis focused on resistance trends and gas index responses to infer response to changes in gas concentration and type. The findings inform the design of cost-effective, scalable sensor technologies for ambient air quality monitoring and environmental resilience applications.

<sup>&</sup>lt;sup>1</sup>Department of Agricultural Economics, Mississippi State University

<sup>&</sup>lt;sup>2</sup>Kansas State University Biological and Agricultural Engineering

### P29\_Disruptions During a Severe Winter Storm: Outages and Impacts Across Kansas' Rural and Urban Communities

Camille Taylor, 1,2 Eliyasu Osman, 1 Jason Bergtold 1

<sup>1</sup>Kansas State University Department of Agricultural Economics <sup>2</sup>Department of Agricultural Economics, Mississippi State University

With the increase in the extent and severity of natural disasters and extreme weather in the past few years, it has become more important to be able to better understand the effects of these storms on different households across communities. We focus on one extreme weather event, a winter storm event that swept across Kansas in January of 2024. The purpose of this research is to look more in depth at the effects of that winter storm on households, such as power and water outages, across rural and urban communities throughout Kansas. By using primary data from a survey conducted in 2024, we use summary statistics to show that rural and micropolitan communities were more susceptible to power and water outages and experienced them for a longer amount of time compared to more metropolitan areas. The information produced is important as it can be used to ensure that emergency response and recovery efforts are adequately addressing the needs of households across different communities, as well as helping to shape policy response for future recovery efforts.

### P30\_Replicating Evidence of Agricultural Spillover Effects in Local Economies

Nick Thompson, 1,2,3 William L. Duncan, 1 and Benjy Jacobs 1

<sup>1</sup>University of Kansas Institute of Policy and Social Research

<sup>2</sup>Kansas State University Department of Statistics

<sup>3</sup>Kansas State University Department of Economics

The Ogallala Aquifer stretches across eight states in the Great Plains region. Following the development of improved irrigation techniques in World War II, it became possible to pump water from wells over the Ogallala Aquifer. This meant that farmers did not have to rely on surface water to irrigate their crops and thus farming became more productive, and more land could be used for farming activities. This project examines whether the advances in agriculture in these communities 'spillover' into non-agriculture sectors, or whether the benefits to the agricultural sector crowd out other areas of economic activity. To do this, the analysis constructs two sets of counties: those largely over the Ogallala Aquifer and nearby counties that do not have significant access to the aquifer. Doing this analysis replicates a study done by Richard Hornbeck and Pinar Keskin in 2015, that showed agriculture negatively affects non-agricultural sectors where the aquifer is present due to increased land prices and disamenities caused by agriculture while not providing enough benefits to offset the costs.

# P31\_A Time Dependent Non-Sequential Monte Carlo Simulation Method for LOLP Computation Under Renewables, Battery and HILF Events

<u>Fayrouz Zeidan</u>,<sup>1</sup> King Nguyen,<sup>2</sup> Adithya Melagoda,<sup>2</sup> Demy Alexander,<sup>2</sup> Visvakumar Aravinthan<sup>2</sup>

The growing integration of intermittent resources, coupled with rising occurrence of High Impact Low-Frequency (HILF) events in recent years, necessitates a reassessment of traditional methods used to calculate reliability indices such as Loss of Load Probability (LOLP). This paper proposes a non-sequential Monte Carlo algorithm which can capture the intermittent behavior of renewables as well as the HILF events effectively. The proposed algorithm is tested on a system with conventional, wind, solar and battery. The sampling technique used for each resource type is performed based on their behavior in different time frames. Simulations carried out utilizing the actual data, resulted in faster computational time as well as better LOLP values compared to the traditional sequential approach. Several test cases were performed to demonstrate this algorithm's speed and accuracy under varying generation conditions.

### P32\_Dehumidification Modeling with Desiccant Wheels

Khue Do<sup>1,2</sup> and Christopher Depcik<sup>3</sup>

<sup>1</sup>Fostering Research Opportunities in Sustainable Technologies (FROST), University of Kansas, Lawrence, KS,

<sup>2</sup>Department of Chemistry, University of Georgia, Athens, GA

The use of desiccant wheels in cooling processes results in a more energy efficient and environmentally friendly dehumidification process. The desiccant, usually silica gel or zeolites, adsorbs water vapor from humid air to produce dry air. Trapped moisture is then evaporated using a separate heated air stream, thus regenerating the desiccant for continuous use. A one-dimensional, isothermal, desiccant wheel model was developed based on the fundamental governing laws of nature: conservation of mass and species. Future work will incorporate conservation of momentum and energy. Governing equations for the model were developed, with source terms incorporated to account for processes not represented by the general governing equations. Source terms for existing models were derived to demonstrate inconsistencies within the literature. The model was implemented in Matlab and validated using experimental data.

<sup>&</sup>lt;sup>1</sup>Louisiana Tech University

<sup>&</sup>lt;sup>2</sup>Wichita State University Electrical and Computer Engineering Department

<sup>&</sup>lt;sup>3</sup>Department of Mechanical Engineering, University of Kansas, Lawrence, KS

# P33\_Phase Equilibria and Thermophysical Properties of Deep Eutectic Solvents with Hydrofluorocarbon Gases

Stephanie L. Dücker, <sup>1,2</sup> Saufishan Thalikkassery Akbar, <sup>3-5</sup> Ana Rita C. Morais, <sup>3-5</sup> and Aaron M. Scurto <sup>3-5</sup> Fostering Research Opportunities in Sustainable Technologies (FROST), University of Kansas, Lawrence, KS, <sup>2</sup>Department of Chemistry, Washington and Lee University, Lexington, VA, <sup>3</sup>Environmentally Applied Refrigerant Technology Hub (EARTH), U.S. National Science Foundation Engineering Research Center, University of Kansas, Lawrence, KS, <sup>4</sup>Wonderful Institute for Sustainable Engineering, University of Kansas, Lawrence, KS <sup>5</sup>Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS

The environmental impact of fluorinated gases (F-gases), widely used in refrigeration applications, has intensified the search for sustainable recovery methods that support a circular economy. Deep eutectic solvents (DESs) have recently emerged as promising alternative absorbents for gas separation due to their lower cost and toxicity compared to conventional absorbents such as ionic liquids. In this study, the solubility of two common F-gases—pentafluoroethane (R-125) and difluoromethane (R-32)—was investigated in DESs based on choline chloride ([Ch]Cl) with Ethylene Glycol of 1:3 molar ratio. The results revealed that R-32 exhibited higher solubility than R-125 across the studied DES systems. The density and viscosity of the pure DES were measured over a temperature range of 25 to 70 °C, and the molar ratios of the synthesized products were confirmed using both ¹H-NMR and ¹³C-NMR analyses. The solubility was measured using the Intelligent Gravitational Analysis (IGA) system and the Phase Equilibrium Transport Properties Apparatus (PETPA). From these results, the competitive selectivity among commercial blends like R410A and DESs is predicted from Henry's constants. R-32 appears to have the highest affinity in DESs. This work continues to support an expanding body of literature on the potential for DESs to serve as an effective refrigerant separation solvent.

### P34\_Ionic Liquid and Hydrofluorocarbons Ternary Systems Equilibria

Kirshaun McGhee, 1-2 Julia E. Espinoza Mejia, 3-5 Mark B. Shiflett, 3-5 and Aaron M. Scurto 3-5 <sup>1</sup> Fostering Research Opportunities in Sustainable Technologies (FROST), University of Kansas, Lawrence, KS 2College of Agriculture, Science, & Technology, Delaware State University, Dover, DE, 3 Environmentally Applied Refrigerant Technology Hub (EARTH), U.S. National Science Foundation Engineering Research Center, University of Kansas, Lawrence, KS, 4 Wonderful Institute for Sustainable Engineering, University of Kansas, Lawrence, KS

The majority of hydrofluorocarbon (HFC) based refrigerants are azeotropic in nature, contain zero ozone depletion potential, and have high global warming potential (GWP). Azeotropic refrigerants are nonrecyclable and hard to separate through conventional distillation. Since refrigerants are in constant demand, it is imperative that new technologies are developed to effectively separate azeotropic refrigerants to support refrigerant recovery and potentially reduce GWP. Emerging technology, such as extractive distillation using an ionic liquid (EDIL), has been used to separate azeotropic HFC-based refrigerants. To optimize this technology, HFC's solubilities in ionic liquids are needed. Most experimental solubility data found in the literature address ideal binary systems. However, EDIL systems operate in a real ternary system. In this study, solubilities from a ternary HFC(1)/HFC(2)/IL(3) system are experimentally measured using a high-pressure and high-temperature variable volume cell (VVC). The VVC system is composed of a high-pressure high-temperature cell, a furnace, a densimeter, and a gas chromatograph (GC). Vapor and liquid equilibrium (VLE) composition of the ternary mixture of two reference HFC solutes, pentafluoroethane (HFC-125) and difluoromethane (HFC-32), and ionic liquid solvent 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [C<sub>2</sub>C<sub>1</sub>im][Tf<sub>2</sub>N] are measured at different pressures (0.1, 0.2, 0.3, 0.4 and 0.5 MPa) and temperatures (25, 30, 40, and 50°C). GC is used to analyze HFC-125 and HFC-32 VLE compositions from the ternary system equilibria. This study will aid in the optimization of the EDIL system and azeotropic refrigerant separation. Recycling and reclaiming refrigerants are essential strategies for reducing the global warming impact of the heating, ventilation, and air conditioning (HVAC) industry.

# P35\_Reducing Cooling Energy & Greenhouse Gas Emissions for Houses Across the United States Through PCM Enhanced Building Envelope and Natural Ventilation

Alborz Nasseri, 1,2 Xu Han, 3 and Youmin Xu 3

<sup>1</sup> Fostering Research Opportunities in Sustainable Technologies (FROST), University of Kansas, Lawrence, KS, <sup>2</sup>Department of Biological Sciences, Northern Illinois University, Dekalb, IL, <sup>3</sup>Department of Civil, Environmental & Architecture Engineering, University of Kansas, Lawrence, KS

As more intense and prolonged heat waves occur across the U.S., residential buildings face growing challenges to maintain comfortable indoor thermal conditions while limiting cooling energy use. This study investigates the performance of phase change material (PCM)-enhanced building envelopes combined with night ventilation as a passive cooling measure for single-family houses. A comprehensive analysis of energy savings and greenhouse gas emissions reduction is conducted across 16 U.S. climate zones. Four cases are simulated and compared: (1) baseline (neither PCM nor natural ventilation), (2) nighttime natural ventilation (NV) only, (3) PCM-only, and (4) combined PCM + NV. Simulations use EnergyPlus and TMY weather files. The baseline is based on DOE prototype single-family houses with DX cooling and gas furnace heating. Models for Cases 2-4 add PCM or NV features. Parametric simulations in Cases 3 and 4 optimize the PCM melting point by climate zone. Results show PCM + NV reduces annual cooling energy by 13.2% to 70.5%, depending on the zone. This hybrid solution provides the greatest energy savings and emissions reduction, demonstrating synergistic benefits. It also sustains safer indoor temperatures, enhancing thermal resilience. In addition to energy savings, emissions reductions include 46.8–561.6 kg CO<sub>2</sub>, 0.000–0.401 kg SO<sub>2</sub>, and 0.042-1.058 kg NO<sub>x</sub> annually. For example, in Miami (Zone 1A), a house saves 561.6 kg CO<sub>2</sub>, 0.141 kg SO<sub>2</sub>, and 0.283 kg NO<sub>x</sub> per year. These findings benefit public health especially for vulnerable populations and support PCM adoption for HVAC downsizing and reduced HFC refrigerant dependence.

#### P36\_Determining the Concentration Limits of Flammability for Low GWP HFCs and HFOs

Nicholas Romano, 1,2 Kevin Turner, 1 and Mark B. Shiflett 1

<sup>1</sup>Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS <sup>2</sup>Department of Chemical Engineering, Texas A&M University, College Station, TX

The phaseout of traditional refrigerants in favor of Hydrofluorocarbons (HFCs), Hydrofluoroolefins (HFOs), and natural refrigerants poses new safety issues for the refrigeration industry. Chlorofluorocarbons (CFCs) and Hydrochlorofluorocarbons (HCFCs) were generally nonflammable, while many HFCs and HFOs can be ignited when concentrated in the correct amounts. Flammable refrigerants will combust and experience continuous flame propagation over a range of fuel% values, the boundaries of which are referred to as the flammability limits. These flammability limits are obtained by sparking a gas mixture, drawing the angle between the electrodes and the edges of the flame cloud. The frame where the cloud is the largest is chosen for this flame angle, and if the angle is 90 degrees, the mixture is at a flammability limit. In addition to flame angle, pressure rise can be measured between the moment before ignition and the highest recorded pressure. Pressure rise is potentially subject to less uncertainty than flame angle due to the lack of human error in measuring values, and could make for a better indicator of refrigerant flammability. To evaluate this, single-component mixtures of R-32 or R-1234yf with air were tested, and the mean and standard deviation were computed for varying concentrations of fuel. From this data, coefficients of variance were found, and the relative uncertainty and dispersion of the data could be determined. The findings from these calculations indicated that with current equipment, flame angle experienced less relative uncertainty and appeared to be a better measure of flammability.

# P37\_Chemical Equilibrium-Based Adiabatic Flame Temperature and Product Prediction for Low-GWP Refrigerants

Adam Smith<sup>1,2</sup> and Christopher Depcik<sup>3</sup>

<sup>1</sup>Fostering Research Opportunities in Sustainable Technologies (FROST), University of Kansas, Lawrence, KS, <sup>2</sup>School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ, <sup>3</sup>Department of Mechanical Engineering, University of Kansas, Lawrence, KS

Global climate regulations necessitate the phase-in of lower global warming potential (GWP) hydrofluoroolefin (HFO) refrigerants. However, the formulation of these refrigerants results in a greater flammability as a trade-off to lowering their GWP. To accelerate an understanding of the combustion behavior of newly developed fluorinated refrigerants and refrigerant blends, a chemical equilibriumbased thermodynamic model for adiabatic flame temperature and pressure that operates under constant pressure or constant volume conditions was developed. The model accounts for initial temperature, pressure, air-fuel ratio, equivalence ratio, and relative humidity, and is refrigerant- and mass-composition general. These parameters make it applicable to a significant number of environmental conditions, including real-world experiments and laboratory testing scenarios. In addition, this model calculates combustion product concentrations as a supporting mechanism, which can be helpful in evaluating the safety of novel refrigerants and refrigerant blends. To quantify the model's accuracy, adiabatic flame temperature values were compared to experimental literature values for several refrigerants and refrigerant blends. Even though the model's complexity is significantly lower than a chemical kinetics-based model, predicted adiabatic flame temperatures are still accurate to within 100 K of experimental data, and can be used as a screening tool for the consideration of new refrigerants and refrigerant blends without any experimental testing or advanced computation.

### P38\_The Effects of Estrogen on the Interfacial Behavior of Myelin Lipid Models

Henry Bair,<sup>1</sup> Estephanie Escobar,<sup>1</sup> Meredith Hartley,<sup>2</sup> and Prajnaparamita Dhar<sup>1</sup> Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS <sup>2</sup>Department of Chemistry, University of Kansas, Lawrence, KS

The myelin sheath is the multilayer lipid membrane wrapped around the axons of neurons in the central nervous system (CNS) that protects nerves and facilitates rapid impulse transmission. Myelin destruction, referred to as demyelination, is observed in Multiple Sclerosis (MS), a neurodegenerative autoimmune disorder resulting in the interruption of nerve signals and consequent loss of motor and sensory functions. Differences in membrane composition have been identified after remyelination; however, the importance of these changes to MS is not yet fully understood. Our previous research has proposed a supporting role for cholesterol in membrane stability. Now, estrogen is another molecule of interest because MS disproportionately presents itself in women. Additionally, physicians have observed more relapses in postpartum and menopause patients, where estrogen levels are lowered, leading us to propose a myelin supportive role for estrogen. Here, we utilized a Langmuir-Pockels trough to measure the surface pressures (SP) of monolayers of healthy and diseased myelin lipid models, subjected to dilatational interfacial stresses. The simplified models used in this work are comprised of estradiol and major myelin lipid components L-a-phosphatidylcholine (PC), L-aphosphatidylethanolamine (PE), L-a-phosphatidylserine (PS), and cholesterol. In these studies, differences in phospholipid head groups alone had minimal effects on the properties of the films. However, the addition of healthy cholesterol amounts helped repair film mechanical properties significantly more than diseased amounts. Furthermore, introducing estrogen into diseased models resulted in significant film condensation consistent with healthy surface activity, suggesting that Estrogen may also play a role in supporting myelin sheath stability.

### P39\_PET Upcycling: CO<sub>2</sub>-Induced Separation of Dicarboxylic Acids from Aqueous Salt Solutions

Cameron T. Burns, 1 Diego T. Melfi, 2,3 and Aaron M. Scurto 2,3

Polyethylene terephthalate (PET), the most widely produced polyester, is derived from fossil fuel-based monomers and suffers from low recycling rates. Chemical recycling via alkaline hydrolysis enables PET to be depolymerized into disodium terephthalate (Na<sub>2</sub>TP) and ethylene glycol (EG), but conventional acidification to recover terephthalic acid (TPA) relies on strong mineral acids like HCI, raising environmental and safety concerns. As a sustainable alternative, carbonic acid was used, generated by bubbling carbon dioxide (CO<sub>2</sub>) into water. These CO<sub>2</sub>-induced precipitations were then applied to aqueous Na<sub>2</sub>TP solutions to obtain TPA. Initial experiments employed synthetic Na<sub>2</sub>TP to isolate the precipitation step, using 1 wt% solutions pressurized with CO<sub>2</sub> to 40 bar. After reacting for two hours, solids were filtered, and NMR analysis was used to calculate removal and vield. Additional studies explored other, more biorenewable, dicarboxylic acids, which were neutralized with NaOH to form disodium salts, and their precipitation behavior was examined under similar conditions. These CO<sub>2</sub>induced precipitations proved effective across multiple acids, achieving yields of >80% for TPA and sebacic acid, and >95% for 2,6-naphthalenedicarboxylic acid (NDA) and 4,4'-bibenzoic acid (BBA). Acids with significantly lower pKa values than carbonic acid, such as 2,5-furandicarboxylic acid (FDCA) and [2,2'-bifuran]-5,5'-dicarboxylic acid (BFDCA), showed minimal yields. Additionally, depolymerization reactions were performed using ground PET and either NaOH or NaHCO<sub>3</sub> in a microwave reactor at 180 °C for 150 minutes. High Na<sub>2</sub>TP (90%) and EG (89%) yields were obtained, consistent across PET loadings and base types. These results highlight CO<sub>2</sub>-induced precipitation as a greener route for acid recovery in PET recycling.

#### P40 Design of an X-ray Transparent Apparatus for HPHT Porous Media Experiments

Oscar Gutierrez<sup>1,2</sup> and Guenther Glatz<sup>1</sup>

This research project investigates the design specifications necessary for an apparatus to conduct *in situ* serpentinization experiments under X-ray computed tomography (CT). Through this research, a custom reactor was developed to maintain X-ray CT transparency while withstanding temperatures up to 350°C and pressures of 4000psi. It is necessary to achieve these parameters while maintaining a compact profile in order to fit the spatial constraints of the X-ray CT system. The utilization of Multiphysics simulation software is essential for optimizing the apparatus's design. The current prototype facilitates X-ray scans with voxel resolutions of approximately 20 microns. Resolution of this quality allows for the improved study of serpentinization within ultramafic rocks. The ability to monitor *in situ* changes in transport and rock mechanics during serpentinization requires technology currently unavailable. An emphasis on tracking fracture patterns within these rocks could allow for the development of predictive models. A comprehensive understanding of serpentinization is essential to commercial geologic hydrogen production.

<sup>&</sup>lt;sup>1</sup>Department of Chemical & Biomedical Engineering, University of Wyoming, Laramie, WY

<sup>&</sup>lt;sup>2</sup>Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>3</sup>Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>1</sup>Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup> Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

### P41\_Rapid Measurement of Interfacial pH by IR-Spectroscopy for Electrochemical Nitrate Reduction

Morgen Keller, Karthik Mamandur Gopalakrishna, and Elizabeth R. Corson Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS

Every year, over a million tons of ammonia is produced to be used in nitrogen-based fertilizers. Through the Haber-Bosch process—the main method of producing ammonia—carbon dioxide (CO<sub>2</sub>) is produced about four times more than the amount of ammonia, polluting the air and massively contributing to climate change. In addition, around 25% of the nitrates within the fertilizer leach into groundwater, polluting it and causing various health issues and heavily damaging aquatic populations. However, by electrochemically reducing nitrate contaminants directly to ammonia, a pollutant is reused, CO2 production is eliminated, and a useful product is formed. While the validity of this reaction has been proven to be effective through electrochemical means, the efficiency and selectivity still needs to be improved to make it a cost-effective solution for the rural communities most effected by groundwater pollution. Specifically, a slightly acidic electrolyte solution has been shown to improve the selectiveness of nitrate reduction to ammonia. Earlier studies have focused on the bulk pH role on selectivity. Our group's previous work has shown that the interfacial pH (10 nm from the electrode surface) changes drastically throughout the reaction. Performing ATR-SEIRAS on an FTIR with rapid scanning capabilities allows analysis of the momentary changes in interfacial pH that would be otherwise undetectable. To ensure accurate interfacial pH measurements throughout the reaction, we calibrated the equipment between 1 to 13 using a phosphate buffer system. Informed by these insights, we aim to enhance the selectivity of nitrate reduction to ammonia.

# P42\_Electrochemical Urea Synthesis from Co-reduction of Nitrate and Carbon Dioxide on an Optimized CuAg Catalyst

<u>Tej Maheshwari,</u><sup>1,2</sup> Mukhtiar Ali,<sup>1</sup> and Elizabeth R. Corson<sup>1</sup>

<sup>1</sup>Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS

<sup>2</sup>Department of Engineering, Brown University, Providence, RI

Despite their high energy demands, the Haber-Bosch and Bosch-Meiser processes dominate industrial urea (H2NCONH2) synthesis. Electrochemical co-reduction of nitrate (NO3-) and carbon dioxide (CO2) offers a sustainable alternative, recycling major air and water pollutants and reducing fossil fuel consumption. However, current catalysts suffer from poor selectivity. We hypothesize a copper-silver thin film catalyst will promote efficient urea synthesis. Prior work indicates copper is an optimal catalyst for reducing nitrates towards ammonia. Silver has been shown to weakly coordinate with carbon dioxide, limiting reduction to carbon monoxide. Together, these two pathways suggest a copper-silver alloy could promote early carbon-nitrogen bond formation, increasing reaction efficiency. We investigate the optimal alloy of silver and copper to maximize the faradaic efficiency of urea synthesis. Alloys are generated through galvanic deposition of silver on copper foils, and the electrochemical reaction occurs in an aqueous flow cell. Reaction intermediates are studied via surface enhanced Raman spectroscopy (SERS) and attenuated total reflectance-surface-enhanced infrared absorption spectroscopy (ATR-SEIRAS). Gaseous and liquid products are characterized via gas chromatography (GC) and nuclear magnetic resonance (NMR), respectively. We hope to find spectral evidence of \*CO2NO2 and lower rates of hydrogen (H2) evolution. These results would improve catalyst design and enhance scientific understanding of electrocatalytic urea synthesis.

### P43\_Phosphorous Recovery from Municipal Sludge Using Hydrothermal Liquefaction

<u>Dylan Maloney,</u><sup>1</sup> Joao Poli, Belinda Sturm, Susan Stagg-Williams

Using municipal sludge as a feedstock for hydrothermal liquefaction (HTL) offers an environmentally friendly and cost-effective way to dispose of wastewater sludge and produce useful products including biocrude oil, biochar, and aqueous co-product (ACP). Some wastewater treatment plants use Enhanced Biological Phosphorous Removal (EBPR) to remove phosphorous from the water fraction of the wastewater. This process utilizes Phosphorous Accumulating Organisms (PAOs) which push phosphate into the water fraction when stored anaerobically and pull phosphate into the solid fraction when stored aerobically. This presentation explores the effects of anaerobic and aerobic storage on the fate of phosphorous in hydrothermal liquefaction products. Previous studies yielded conflicting results, so SEAL Analytics was used to test the orthophosphate levels of both old studies and current wastewater. This helped to reveal the effect of EBPR being inoperative on phosphorous yields in the biochar and ACP. Current sludge and HTL products will be tested using an Inductively Coupled Plasma (ICP) machine in order to reveal more of their molecular makeup. This research also lays the groundwork for future studies concerning the use of hydrothermal liquefaction to break down Polyfluoroalkyl Substances (PFAS) and PFAS precursors.

### P44\_Catalytic Cracking of Polyethylene under Subcritical CO<sub>2</sub> as a solvent

Tifiani Palm, 1,2 Nicholas Gorschak, 1 and Ana Morais 1

An alternative to the traditional recycling of polyolefin waste is converting it to hydrocarbon fuels, but this approach faces mass transfer limitations. In this work, we explore the use of CO<sub>2</sub> as a reaction medium for the catalytic hydrocracking of polyethylene into lower-order hydrocarbons in the range of fuels such as gasoline and diesel. 5 wt% Ru/H-Beta or Ru-HY were investigated as catalysts, and the reaction conditions used to crack the polyethylene were 200°C for 4 hours. Each reaction was run in the presence of 30 bar of H<sub>2</sub> and varying pressures of CO<sub>2</sub>, and the ideal CO<sub>2</sub> pressure out of those tested was determined to be 30 bar. The results show significant improvements in conversion rates and liquid yields, with an increase of 66% and 27%, respectively, from the control reactions conducted with H<sub>2</sub> only. A shift towards more isomerized products for both catalysts was observed with increasing pressure. We can conclude from this data that using CO<sub>2</sub> as a solvent for catalytic hydrocracking has several benefits for the conversion of polyolefins into hydrocarbon fuels.

<sup>&</sup>lt;sup>1</sup>Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS <sup>2</sup>Department of Civil & Environmental Engineering, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>1</sup>Wonderful Institute for Sustainable Engineering, University of Kansas, Lawrence, KS <sup>2</sup>Department of Engineering, University of Tulsa, Tulsa, OK

### P45\_Uncovering Mass Transport Effects in Pd-Catalyzed Cross Coupling:

Pritam Ray, Thomas Gonzales, and Alan Allgeier

Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS

The Suzuki-Miyaura Cross-Coupling (SMC) reaction is utilized to form selective carbon-carbon bonds for the synthesis of complex molecules and has a multitude of applications ranging from agrochemicals. pharmaceuticals, technology such as OLEDs, and even flavonoids. In this research, phenylboronic acid and 4-bromobiphenyl react together in the presence of solid potassium carbonate as the base and XPhos-Pd G2 as the catalyst to form para-terphenyl in methyl-tetrahydrofuran as the solvent. This research aims to bypass the mass transport limitations which arises due to the presence of the solid base and its impact on the performance of our specific reaction. To examine the mass transport affect and the kinetic behavior, we vary the base particle size from <38 µm to 100-425 µm, temperature at 35°C, 45°C, & 75°C, and orbital & stir bar mixing regimes. Reaction samples were processed through High Pressure Liquid Chromatography (HPLC) in combination with UV-Vis to determine the absorbance of the reactants and products throughout the duration of the reaction. In combination with linear calibrations and the absorbance data gathered from HPLC/UV-vis chromatography for each analyte, the concentration was determined for any given time. This research concludes particle size and mixing regimes play a significant role in the impact of mass transport effects on the SMC reaction in the presence of a solid base. These insights showcase the importance of mass transport limitations associated with a solid base and emphasizes the role of the base in the SMC reaction.

### P46\_Polymeric Membranes for Refrigerant Separation

Anna Rosu, 1,2 Yuniva Mendoza Apodaca, 1 and Mark B. Shiflett 1

<sup>1</sup>Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS <sup>2</sup>Department of Materials Science and Engineering, University of Wisconsin Madison, Madison, WI

The increasing environmental regulations on hydrofluorocarbon (HFC) emissions and the need for efficient refrigerant recovery technologies have driven interest in membrane-based gas separation for the recovery and reuse of refrigerant gases. This study focuses on the fabrication of high-performance polymeric membranes designed for the selective separation of refrigerant gas mixtures. The membranes were synthesized using N-Methyl-2-pyrrolidone (NMP) as a solvent and a combination of 6FDA (4,4'-(hexafluoroisopropylidene)diphthalic anhydride) and TrMDP (2,4,6-trimethyl-1,3-diaminobenzene) as monomers. A solution casting technique was employed under controlled conditions to optimize polymer chain formation and membrane uniformity. The fabricated membranes demonstrate promising structural integrity and thermal stability, making them strong candidates for gas separation applications. To evaluate their practical effectiveness, the membranes will be tested for their permeability and selectivity using HFC-125 and HFC-32, two commonly used refrigerants in commercial blends such as R-410A. Future work will focus on characterizing these gas transport properties and assessing the membranes' separation performance for these refrigerant gas pairs.

# P47\_Effects of Polyfluoroalkyl Substances (PFAS) on the Lung Surfactant Component Dipalmitoylphosphatidylcholine (DPPC)

Ananya Saravana, 1,2 Abdullah Al-Raigi, 1 and Dr. Prajnaparamita Dhar 1

<sup>1</sup>Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS <sup>2</sup>Department of Chemical Engineering & Bioengineering, Washington State University, Pullman, WA

Polyfluoroalkyl substances (PFAS) are synthetic chemicals found in a wide range of consumer products and are present in both indoor and outdoor air. When inhaled, PFAS can reach the alveoli, which are small air sacs in the lungs responsible for gas exchange. Within the alveoli, there is an air-liquid interface where surface tension occurs. Excessive surface tension can lead to alveolar collapse, reducing the surface area available for oxygen exchange. To prevent this, the lungs produce surfactants, which are partially composed of dipalmitoylphosphatidylcholine (DPPC), that reduce surface tension close to zero, allowing for full alveolar expansion. The effect of PFAS on lung surfactant function is not well understood, especially how different types and concentrations of PFAS alter surfactant performance. In this study, a Langmuir trough was used to simulate five breathing cycles, modeling the compression and expansion of alveoli. The subphase was prepared using a buffer with a pH similar to alveolar fluid, and varying concentrations of two PFAS compounds, perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS), were introduced. DPPC was then spread on the surface, and surface pressure was measured to evaluate the interaction between PFAS and lung surfactant. The results show that both PFOA and PFOS decreased in maximum surface pressure as concentration increased, meaning that surface tension was unable to be reduced to zero. PFOA reduced surface pressure more than PFOS at increasing concentrations. The compressional modulus results, which indicate film stability, for PFOS were smaller than PFOA at increasing concentrations.

# P48\_Valorization of Biomass Derivatives to Monomers by M-MO $_{\rm x}$ Catalytic Hydrogenation & Hydrodeoxygenation

William Steere, 1 Samir F. Castilla-Acevedo, 2 and Alan M. Allgeier 2

- <sup>1</sup> Department of Chemical and Bioengineering, University of New Hampshire, Durham, NH
- <sup>2</sup> Center for Environmentally Beneficial Catalysis and Chemical & Petroleum Engineering Department, University of Kansas, Lawrence, KS

With increasing concern regarding global warming contributions by fossil fuels in petrochemical production, the potential use of biomass-derived molecules to serve as a more eco-friendly feedstock has grown in popularity. Specifically, sebacic acid, a versatile chemical used to produce nylons, plasticizers, and lubricants, has the potential to be obtained from bio renewable feedstocks and alleviate environmental drawbacks from fossil fuel petrochemical production. Our research validates the catalytic conversion of the biomass-derived 2,2'-bifuran 5,5'-dicarboxylate (BFDCM) to sebacic acid (SA), through M-MO<sub>x</sub> catalyzed hydrogenation and hydrodeoxygenation. Catalytic activity tests were conducted for 4 different 5% wt. Pd-supported catalysts (C, Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, and TiO<sub>2</sub>) to understand the role of temperature in the ring hydrogenation of BFDCM. Gas Chromatography coupled with Mass Spectrometry (GC-MS) was used for identification and quantification of products. CO-Pulse chemisorption was employed to examine Pd dispersion on the support surface. Commercial 5% wt Pd/Al2O3 reacted at 60°C and 3 MPa H<sub>2</sub> as initial pressure for 2 hours outperformed others with hydrogenation conversion and selectivity greater than 95% along with maintaining product purity above 98%. Notably, reactions with Pd/Al<sub>2</sub>O<sub>3</sub>, Pd/C, and Pd/TiO<sub>2</sub> at high hydrogenation reaction temperatures (≥100°C) experienced wider product distributions. These novel catalytic processes provide direction for establishing an environmentally friendly circular economy within the chemical and agricultural industries while incentivizing developments in green petrochemical syntheses.

# P49\_Production of Jet Fuel Range Liquid Alkanes from One-Pot Synthesis by Transition and Noble Metal Loaded Acidic Hierarchical H-Y Zeolites

<u>Isaiah True</u>,<sup>1,2</sup> Kingsley Siakpebru,<sup>1,2</sup> Monte Asisian,<sup>1,2</sup> Ana Rita C. Morais<sup>1,2</sup>

<sup>1</sup>Wonderful Institute for Sustainable Engineering, University of Kansas, Lawrence, KS

<sup>2</sup>Department of Chemical & Petroleum Engineering, University of Kansas, Lawrence, KS

The efficient conversion of lignocellulosic biomass into renewable fuels remains a critical challenge due to the high energy consumption and complexity of existing methods. To overcome these limitations, a new catalyst modification was developed for the direct conversion of lignocellulose to jet fuel and diesel range alkanes. Na-Y zeolites were engineered into H-Y hierarchical zeolites, significantly increasing both pore size and surface area, enhancing catalyst accessibility and activity. Furthermore, transition and noble metals were incorporated onto these acidic hierarchical H-Y zeolite catalysts, with a focus on achieving reduced particle sizes to maximize catalytic performance. These modified catalysts effectively promoted hydrogenation and hydrogenolysis reactions, enabling the one-pot synthesis of C8-C15 alkanes and aromatics with high selectivity. When applied to poplar biomass, this catalyst achieved a 47.3 wt% conversion rate, with high selectivity towards the target components: 35% for C8 cycloalkanes and 45% for C9 cycloalkanes. This approach offers a promising, potentially scalable pathway for sustainable biofuel production, addressing the demand for greener transportation fuels.

### P50\_Impact of Bile Acid Hydroxylation State on Cyclic Peptide-Micelle Interactions

Alan Bernstein, 1,2 Maryann Melendrez, 1 Zahraa Al-Tamimi 1, and Michael Hageman 1 Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS 2 Department of Chemistry, Boston University, Boston, MA

Peptide drugs are a rapidly growing therapeutic class due to their high specificity, potency, and predictable metabolism. However, their chemical structure presents key challenges for oral delivery, including poor enzymatic stability and low gastrointestinal (GI) membrane permeability. In the duodenum, bile acids (BA) and phospholipids (PL) form mixed micelles that interact with peptide drugs to influence solubility, stability, and absorption. A major factor governing these interactions is the BA hydroxylation state, which modulates micelle formation through hydrophobic effects and hydrogen bonding. The impact of BA hydroxylation on peptide flux and enzymatic degradation remains poorly defined. To address this gap, we evaluated the membrane flux and stability of a cyclic peptide (i.e., octreotide) and three monosubstituted analogs (A4, A5, D5) in the presence of trihydroxy (NaTC) and dihydroxy (NaTDC) BA. Flux was consistently higher in NaTC/PL than NaTDC/PL across all peptides, suggesting that reduced hydroxylation increases peptide-micelle interactions and limits flux. Octreotide showed low flux in both media, consistent with strong micelle association, while D5 exhibited high flux (thus minimal association). A4 and A5 showed moderate flux, indicating that their substitutions attenuated but did not eliminate micelle interaction. Enzymatic stability was modestly improved by BA/PL micelles for octreotide and A5, with no substantial difference between NaTC and NaTDC. D5 remained stable in all conditions, suggesting limited enzyme interaction independent of micelle effects. These findings support a tradeoff between micelle-mediated protection and flux, and highlight the importance of both BA structure and peptide modifications in tuning oral bioavailability.

### P51\_Impact of Hydrophobic Antioxidants on Oxidation Prevention of Methyl Linoleate

<u>Jake G. Ferguson</u>, Sheryhan F. Gad, Indeewara Munasinghe, Michael J. Hageman Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

The importance of unsaturated lipid-based formulations in improving solubility and bioavailability of poorly soluble drugs is significant. Yet there are many challenges to working with unsaturated fatty acid like excipients and APIs due to autoxidation followed by further degradation reactions. This leads to safety and efficacy compromises in the drug product. The goal of this project was to test the effects of different hydrophobic and amphipathic antioxidants on the inhibition of oxidation of Methyl Linoleate (MLO), a model drug for fatty acid-like API's and excipients. MLO was stored at 6 °C, 25 °C, and 40 °C at 2% antioxidants and at varying antioxidant concentrations up to 21 days. The exposed MLO solutions were then analyzed using a developed UPLC method. The results so far show that hydrophobic antioxidants readily prevent oxidation (<1% oxidation) at all storage conditions, while amphipathic antioxidants show moderate oxidation prevention (up to 25% oxidation). MLO without antioxidants showed 15%, 30%, and 60% oxidation levels at 6 °C, 25 °C, and 40 °C, respectively, in 10 days. The results also show that higher concentrations of antioxidants were not always more effective at preventing oxidation.

#### P52\_Stability of Nitroglycerin Sublingual Tablets: Impact of Packaging and Storage

Adriana Gallegos, Monica Whalen, Sheryhan F. Gad, Yezan Salamoun, Michael Hageman Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

Sublingual Nitroglycerin is a first line therapy used to treat angina and cardiac emergencies. These tablets, although practical, have their own set of challenges tied to its stability. NTG tablets are easily prone to degradation through many pathways because of its sensitivity to heat, humidity, and light, plus its volatile nature. To prevent degradation, NTG tablets are stored in an amber glass vial at 20°C-25°C, in counts of 25 or 100 tablets. This creates an issue within an inpatient setting where many oral medications are packaged separately in unit-dose packaging. NTG cannot currently be stored in these packages because they must be kept inside their original container. For that reason, each time a vial is opened to air, the tablets are prone to degradation through oxidation. The objective of this study is to understand the stability of NTG under certain conditions in unit-dose packaging versus multi-dose packaging.

### P53\_Characterization of Liposomal Properties: A Molecular Dynamics Approach

Hamza Habib, 1,2 Hashim Mushtasin Reza1, and Hao Lou1

<sup>1</sup>Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

Liposomes offer a versatile platform for subcutaneous delivery of small molecule therapeutics, formulations of which can be tailored to influence release kinetics and stability. Very little literature exists on using molecular dynamics to evaluate liposomal formation and physiochemical properties as a function of formulation. In this study, we explore liposomal systems composed of various amounts of 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC), cholesteryl hemisuccinate (CHEMS), and PEGylated lipids (DSPE-PEG2000); these liposomes will also be loaded with dexamethasone and ibuprofen separately as model drugs. Employing coarse-grained molecular dynamics simulations, we explore the self-assembly and structural properties of liposomes for each formulation. Our results show that increasing CHEMS concentration leads to more compact liposomal morphology but total sphericity is insensitive to composition. These findings highlight the significance of lipid formulation in regulating both loading efficiency and release behavior, and provide molecular-level insight for rational liposome design specific to controlled drug release.

### P54\_Modulating Precipitation of Small Molecule Drugs Following Intraperitoneal Injection

<u>Josephine Herrold</u>, Jack Terry, Michael Hageman Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

The intraperitoneal cavity has a strong vascular and lymphatic network allowing for prompt drug absorption. It houses major internal organs and contains fluid derived from surrounding interstitial cells. The fluid dilutes excipient formulations upon administration and provides modest buffering. IP drug administration is typically utilized for pre-clinical development in stages where multiple analogs must be evaluated guickly, leading to minimal formulation optimization. We have developed a model drug formulation system which allows for the observation of precipitation upon dilution levels expected from IP administration. The formulations combine Captisol, a cyclic molecule of seven dextrose units, and PEG 300, a low-toxicity liquid polymer. Celecoxib is a small molecule drug that has poor aqueous solubility (BCS Class 2). To measure the solubility of Celecoxib, a calibration curve was devised and quantified by a UPLC. A matrix of excipient formulations was prepared, excess drug added, and supernatant was sampled and assayed. For the second method, a high-concentration PEG stock was made and added to the associated Captisol formulation to induce precipitation. Both methods had similar results indicating that precipitated Celecoxib shares the same crystalline habit as the commercial solid. We also measured visible light occlusion following a simulated IP injection to quantify precipitation speed. Higher Captisol concentrations occluded less visible light upon precipitation and higher PEG 300 formulations led to greater variation reducing the effect of Captisol, which indicates that Captisol can modulate precipitation. Future experiments will include in-vitro micro dialysis, side-byside diffusion, and in-vivo administration. These will assess how drug complexation with Captisol affects permeation and bioavailability.

<sup>&</sup>lt;sup>2</sup>Department of Chemistry, Wesleyan University, Middletown, CT

### P55\_HEADSPACE ANALYSIS OF HALOGENATED SOLVENTS IN SOLUTION

Zachary Logan, 1,2 Indika Warnakula,1 and Michael Hageman1

<sup>1</sup>Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

Headspace analysis is a gas chromatographic technique that is used to detect volatile or semi-volatile organic compounds in a sample. In the context of pharmaceutical chemistry, this technique is used to determine the presence and identity of any residual volatile solvents that may remain in a drug formulation post-synthesis. This project focuses on the headspace analysis of halogenated solvents in solution together, a topic that has previously not been studied. Furthermore, this study also involves investigation of stirring, pH, and surfactant addition effects on the presence of these solvents in the headspace. The column conditions for this study were optimized from previous methods and the sample preparation involved the preparation of samples in crimp sealed amber vials to prevent headspace loss. Sample injection was done via a solid-phase micro-extraction (SPME) probe, which absorbs gaseous species present in the headspace. It was determined that chloroform and bromoform are in competition with one another for room in the headspace, this was confirmed by seeing lower peak areas when in a mixture sample. It was also found that both stirring, and surfactant addition decreased the concentration of bromoform in the headspace. Chloroform was generally seen to have sporadic trends, and it would be worthwhile to study further.

# P56\_Assessing the Effect of Phospholipid Concentration in Bile Salt Mixed Micelles and their Interaction with Cyclic Oral Peptide Drugs

Maryann L. Melendrez Cuadros, 1,2 Alan Bernstein, 2 Zahraa Al-Tamimi, 1 and Michael Hageman 1

<sup>1</sup> Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

Peptides are emerging as powerful therapeutic agents in a wide range of clinical applications. Despite significant advancements in their development, their oral delivery remains limited due to enzymatic degradation, poor permeability, and low bioavailability. Previous research has shown that mixed micelles composed of bile salts (BS) and phospholipids (PL) have a negative influence on peptide absorption. However, the influence of micelle composition, especially PL concentration, on peptide transport mechanisms is not fully understood. This study investigates how variations in taurocholate (NaTC) and PL ratio affect the interaction, stability, and flux of cyclic peptide analogs, using side-byside diffusion cells and enzymatic degradation assays. Cyclic analogs of octreotide were evaluated under varying micellar environments. Results revealed that peptides with stronger micelle interactions. via electrostatic and hydrophobic forces, demonstrated lower flux but improved enzymatic stability. Moreover, a 2:1 NaTC:PL ratio significantly prolonged half-life in select analogs. To interpret these effects, we developed an initial regression model correlating flux with molecular descriptors (e.g., LogD, pKa) and media properties (e.g., micelle size). We also implemented a preliminary compartmental ordinary differential equation (ODE) model to simulate free fraction, degradation, diffusion, and absorption, serving as a basis for a more refined predictive tool. Future work will focus on optimizing this model to better capture the complex dynamics of micelle-peptide systems.

<sup>&</sup>lt;sup>2</sup>Department of Chemistry and Biochemistry, Southwestern University, Georgetown, TX

<sup>&</sup>lt;sup>2</sup> Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>3</sup> Department of Chemistry, Boston University, Boston, MA

# P57\_Expression and Characterization of an Essential Cytochrome P450 Enzyme of *Leishmania Donovani* for Crystallography

<u>Jason Meschke</u>, Lingli Qin, Deepak Timalsina, Mounika Katamneni, and Michael Wang <sup>1</sup>Department of Chemistry, University of Kansas, Lawrence, KS

Leishmaniasis is a lethal disease caused by a protist parasite, with no approved vaccine, emerging drug resistance, and a 95% fatality rate when untreated. The cytochrome P450 enzyme CYP5122A1 is essential for ergosterol biosynthesis in Leishmania and presents a promising drug target. Although its structure could be elucidated by x-ray crystallography, crystallization has been challenging. In silico models such as AlphaFold fall short in accurately predicting ligand affinities and mutational effects. To promote crystallization, we substituted four surface lysines with alanines to reduce entropy loss during crystal formation. The mutant CYP5122A1 was heterologously expressed in IPTG-induced E. coli, and lysed cells were purified via Nickel-NTA chromatography. Fractions containing the target protein were identified by CYP450's characteristic absorbance peaks at 420 nm and 450 nm. Heme incorporation was confirmed via CO-induced spectral shift, yielding a spectrophotometric index of 1.23. While protein quantification by BCA assay is complete, crystallization is pending further purification through size exclusion and ion exchange chromatography, followed by western blot validation.

### P58\_Screening of Immunomodulatory Drug Candidates for Gastrointestinal Immunotherapy

Austin Petfalski, 1,2 Grahmm Funk, 1 Hyunjoon Kim1

<sup>1</sup>Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

Gastrointestinal (GI) immunity defends the GI tract, and ultimately the whole body, from ingested foreign agents and pathogens. Activation of GI immune cells exhibits a fine balance between too much and too little activity, which can lead to problems like ulcerative colitis1 or infections2. This project aims to identify compounds that can aid GI immunity by stimulating the immune system. The drug candidates presented here were first identified by an NF-kB reporter cell line, confirming their ability to activate a transcription factor common to many immune responses. To gain further insight into their immune activity, bone marrow dendritic cells (BMDCs) treated with the drug candidates underwent flow cytometry and ELISA experiments. With these methods, we were able to characterize the immunogenicity of each drug candidate. Altogether, understanding of these drugs' immunogenicity will help reveal new drug candidates to prime the immune system.

<sup>&</sup>lt;sup>2</sup>Department of Biochemistry, Biophysics, and Molecular Biology, Iowa State University, Ames, IA

### P59\_Regulation of Autophagy Flux by Metformin: Insights into Molecular Pathway

Udita Shah, 1,2 Thuraya Mutawi, 1 and Carlo Barnaba.1

Metformin is a widely used antidiabetic drug also associated with anti-cancer and anti-aging effects, often thought to act through activation of autophagy via the AMPK signaling pathway. Our lab has recently demonstrated that activation of AMPK – the main cellular energy sensor – causes inhibition of autophagy, rather than its activation. Thus, we hypothesize that metformin activation of AMPK may have a different role in autophagy regulation. To prove our hypothesis, we used both western blots (WB) and fluorescence microscopy. WB shows that metformin causes dose-independent inhibition of LC3 accumulation, indicating autophagy inhibition. Similarly, P62 degradation seems not to be promoted. Using live-cell imaging with endogenously Halo-tagged autophagy proteins WIPI2 (Halo-WIPI2), further edited to express a GFP version of the autophagy marker P62 (GFP-P62), we tracked autophagosome formation at the single-cell level. We observed that metformin does not induce autophagy under conditions of AMPK activation with glucose starvation. These results suggest that metformin, via AMPK activation, may prevent phagophore initiation, thereby inhibiting autophagy flux. Our findings challenge the traditional view of metformin as a universal autophagy activator and highlight the complexity of autophagy regulation under metabolic stress.

### P60\_Design and Synthesis of Lipophilic Mycosamine-Modified Amphotericin B Prodrugs

Colin Silva, 1,2 Mikayla Smith-Craven,1 and Michael Hageman1

Amphotericin B (AmB) remains the gold-standard antifungal for invasive mycoses, yet its poor oral bioavailability limits it to intravenous administration. One promising strategy for developing a oral formulation of AmB is prodrugging the primary amine on the mycosamine ring to increase lipophilicity and improve gastrointestinal permeation. Here we report the design and initial synthetic exploration of a lipophilic C14 mycosamine-modified AmB prodrug (denoted AmB-O14). 1-Tetradecanol was converted to its N-hydroxysuccinimide carbonate with disuccinimidyl carbonate in anhydrous DMF (r.t., 16h). After sequential liquid-liquid extractions (0.1 M HCl/brine, sat. NaHCO<sub>3</sub>, brine) and drying, the activated ester was isolated in 83% yield. Coupling to AmB (600 mg, 0.65 mmol) in 2:1 DMF/DMSO, (r.t., 4h) selectively modified the C-3' amine, yielding 486 mg crude C14 carbamate (0.42 mmol, 71% of theory). Analytical RP-HPLC (C18, isocratic 77% ACN/23% H<sub>2</sub>O + 0.2% acetic acid, 16 min) shows a 14 min retention-time shift relative to parent AmB, consistent with the predicted rise in hydrophobicity. Comprehensive 2D NMR assignment is under way; preliminary <sup>1</sup>H data suggests downfield shifts for H-2'/H-3', supporting carbamate formation, though full spectral assignments are not yet complete. These results validate mycosamine-directed lipophilic modification as a tractable synthetic entry point and provide a reproducible workflow for the planned library of lipophilic AmB prodrugs now in progress.

<sup>&</sup>lt;sup>1</sup>Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup>Department of Molecular Biosciences, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>1</sup>Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

<sup>&</sup>lt;sup>2</sup>Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS

### P61\_Evaluating Thermal Stability of Sublingual Nitroglycerin Tablets

Monica Whalen, Adriana Gallegos, Sheryhan F. Gad, Yezan Salamoun, and Michael Hageman Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS

Nitroglycerin is a nitrate and serves the purpose as a vasodilator. Nitroglycerin relaxes and expands blood vessels to help improve blood flow and reduce the hearts workload. Nitroglycerin is a volatile substance which is why the medication works quickly, but that is its downfall. Our purpose is to study the stability of nitroglycerin at different temperatures and conditions.

Nitroglycerin tablets were placed in two different temperature conditions, both contained tablets in open and closed vials. Using UPLC and 100% nitroglycerin in ethanol a standard curve was generated. The standard curve was used to calculate drug degradation. In all trials 60:40 MeOH in H2O was used to dissolve the tablets. At each time point two tablets were analyzed and the average drug concentration was taken. Our study was conducted over 1 month at various time points. For the tablets tested at 25° C, both open and closed containers had little to no degradation and the graph remained linear. The closed vial tablets held at 40° had a similar trend as those held at 25° C and we saw little drug degradation. The tablets in the open condition at 40° did degrade over time and by week one the tablets had lost 20% of drug, by 1 month they lost 70% drug. Thermal stability was tested using thermogravimetric analysis. Each tablet was placed at a set temperature and held at isotherm for one hour. The results showed that as temperature increased weight loss increases, but a small percentage is from the drug.