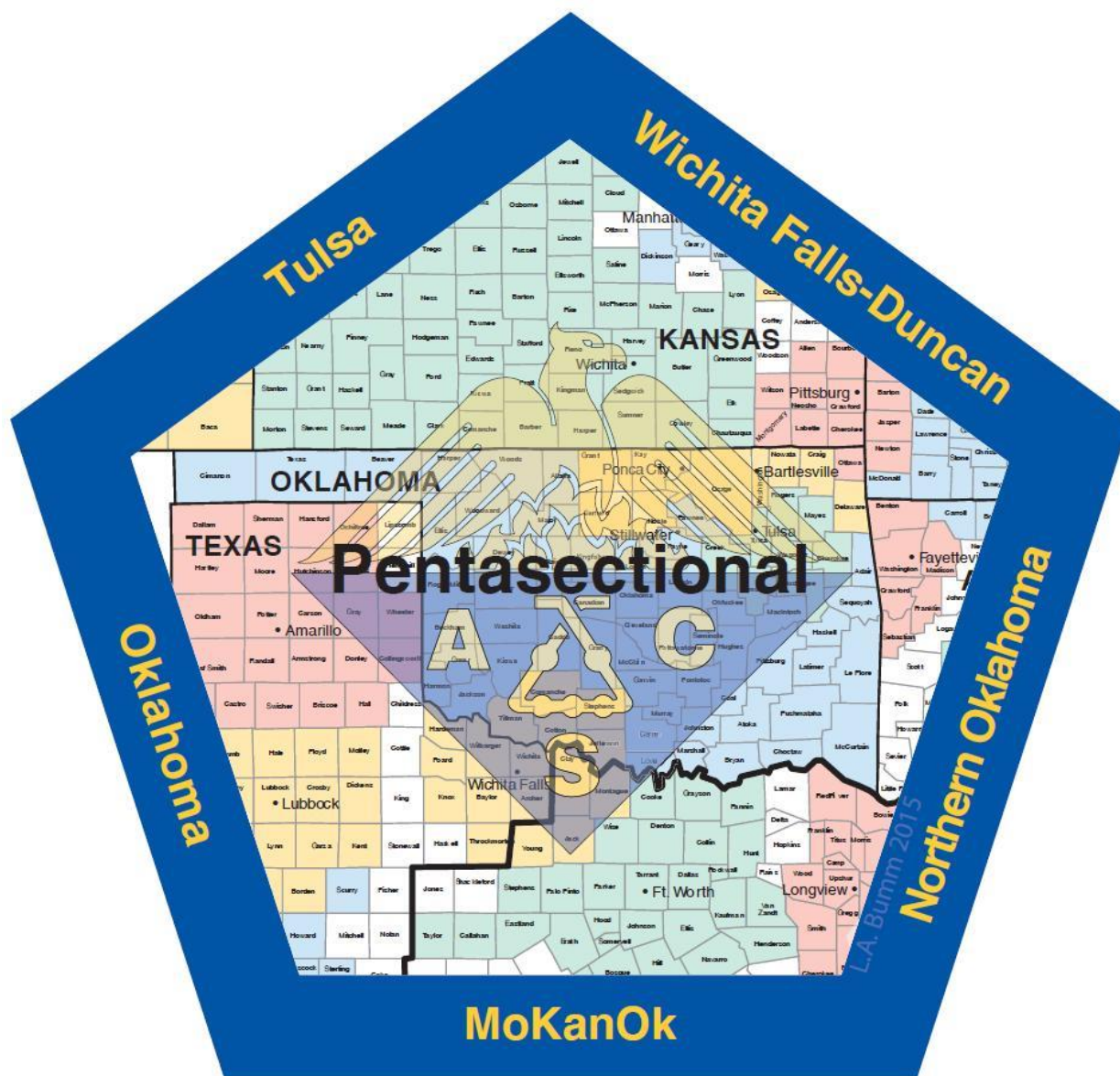


65th Annual Pentasectional Meeting in Bartlesville, OK October 8, 2022



Sustainable and Transformative Chemistry

Acknowledgements

NOKACS acknowledges and appreciates Phillips 66 and Chevron Phillips Chemical Company for their support to the organization of the 65th Pentasectional Meeting.

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Venue

Friday evening Social, Friday, October 7, 2022, 5:30-9:00pm

Woolaroc Ranch

Attention: The gate will close at 7:00pm. Please plan your arrival accordingly.

65th Pentasectional Meeting, Saturday, October 8, 2022

Phillips 66 Research Center

Hwy 60 & 123

Bartlesville, OK 74003

Organizing Committee

General Co-Chairs of the Pentasectional Meeting:

- Dr. Masud Monwar (2022 NOKACS Chair, Chevron Phillips Chemical Company), Email: monwam@cpchem.com
- Dr. Raj Kailasam (Phillips 66), Email: raj.kailasam@p66.com

Program Chair and 2022 OKACS Chair:

- Dr. Jeanne L. Bolliger (Oklahoma State University), Email: jeanne.bolliger@okstate.edu

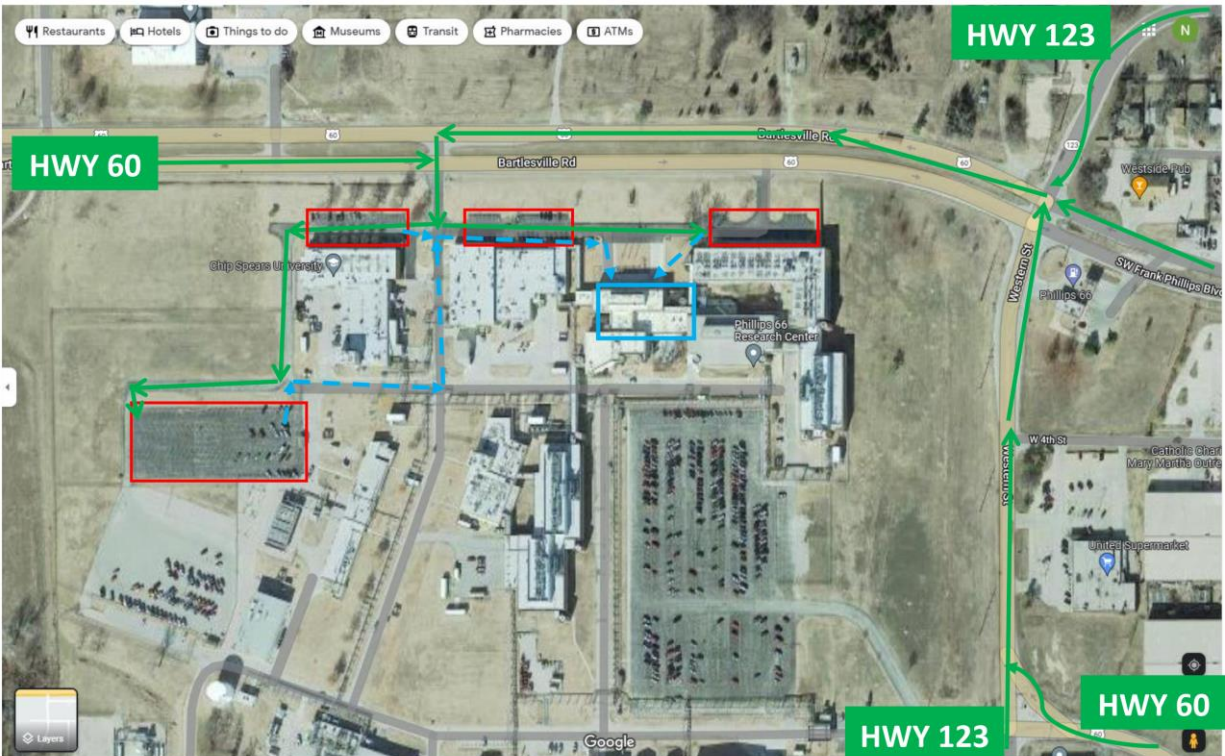
Friday Social Event Coordinator:

- Dr. Randy Heald, Email: randyheald@icloud.com

Program Overview

| | | | | | |
|---------------------|--|--------------|------------------------------------|-----------------------|----------------|
| 7:00am | Venue opens/Check-in (Flagpole Entrance of Phillips 66 Research Center) | | | | |
| 7:30-8:15am | Breakfast (Cafeteria) | | | | |
| 8:30-9:30am | Hall 1: General Morning Session Welcome, Safety, Keynote Talk, Announcement of Oklahoma Chemist of the Year | | | | |
| 9:30-9:50am | Coffee Break (Cafeteria) | | | | |
| Concurrent Sessions | Hall 1 | Hall 2 | Conf Room 1 | Conf Room 2 | Conf Room 3 |
| 9:50-11:30am | Polymer I | Organic | Physical/Computational & Inorganic | Chemical Education I | (for meetings) |
| 11:40am -1:00pm | Lunch, Career Talk with Industry Leaders, Section Chairs Meeting | | | | |
| 1:00-2:30pm | Poster Session (Cafeteria) | | | | |
| 2:00-3:00pm | Coffee Break (Cafeteria) | | | | |
| Concurrent Sessions | Hall 1 | Hall 2 | Conf Room 1 | Conf Room 2 | Conf Room 3 |
| 2:30pm - 4:30pm | Polymer II | Biochemistry | Energy & Environment | Chemical Education II | Analytical |
| 4:40 - 4:50pm | Hall 1: Concluding remarks | | | | |

Parking Directions



Legend:
[Red Box] Parking Allowed [Green Arrow] Driving Direction
[Blue Box] Meeting Venue [Blue Arrow] Walk to Meeting Venue

DIRECTIONS TO THE PHILLIPS 66 RESEARCH CENTER:

Enter 'Phillips 66 Research Center' in Google maps for direction. If you can enter the name the way mentioned here, Google map will show the correct location of the venue. Follow the directions of the Google map and the parking signage once you enter the facility.

OR

1. If you are coming from the South (i.e., Tulsa area), take US-75 North to "Bartlesville".
2. US-75 becomes Washington Boulevard after entering Bartlesville city limit. At the intersection of US Hwy 60, head west toward Pawhuska/Ponca City.
3. When US Hwy 60 intersects State HWY 123 (Western Street), at stoplight turn North/right on State Hwy 123/Western Street. Drive to four-way stop, turn left and follow US Hwy 60 west toward Pawhuska. At first break in divided highway turn left into Phillips 66 complex.
4. After entering the complex, follow signs to the parking lot (red boxes in the map above).
5. Park your vehicle and walk to the building entrance near the flagpoles (dotted blue lines in the map above). If you need help, please talk to the security personnel.
6. At the entrance, present your photo ID to security personnel to prove your identity and conference registration. Security personnel will need to check your backpacks and poster holders. Please be patient and cooperate with the security personnel.

Important Note: Phillips 66 Research Center is a secured facility and safety of the personnel and venue always takes priority!

Detailed Scientific Program

- 7:00am Venue opens
- 7:30-10:30 am Registration/Check-in/Badge and name tag pick up
- 7:30-8:15am Breakfast (Cafeteria)

8:30-9:30am: General Morning Session (Hall 1)

- 8:30-8:35am Welcome (Dr. Masud Monwar)
- 8:35-8:40am Venue Safety Briefing (Mr. Bryan Anderson, Shift Superintendent, Phillips 66)
- 8:40-9:20am Introduction of Keynote Speaker (Dr. Masud Monwar)
- Keynote Lecture by Dr. Mitchell D. Refvik (Abstract T1)
Developing Circular Solutions in the Petrochemicals Industry
Mitchell D. Refvik, Senior Manager Polyolefin Catalysis, Chevron Phillips Chemical Company LP
- 9:20-9:30am Announcement of the Oklahoma Chemist of the Year (Dr. Nathan Green/Dr. Raj Kailasam)
- 9:30-9:50am Coffee Break (Cafeteria)

9:50-11:30am: Concurrent Scientific Talks

Hall 1 (Polymer I), Hall 2 (Organic), Conference Room 1 (Physical/Computational and Inorganic), Conference Room 2 (Chemical Education I)

Polymer Chemistry I (Hall 1)

Session Chair: Dr. Mitchell D. Refvik

- 9:50-10:10am **Post-consumer polypropylene carpet and mixed polyolefin waste make structural composites (Abstract T36)**
*Anuj Maheshwari, Mohamadreza Youssefi Azarfam, Siddhesh Chaudhari, Clinton Switzer, Jay C. Hanan, Sudheer Bandla, Ranji Vaidyanathan, Frank D. Blum**
- 10:10-10:30am **Plant-based Polyol and further Polyurethane/ Graphene-based Composites to Study the Increasing Mechanical Strength (Abstract T37)**
Vishwa Suthar, Magdalene A. Asare, and Ram K. Gupta
- 10:30-10:50am **One Pot Phenolic-Initiated Mechanochemical Synthesis of Poly(lactic acid) Nanoparticles (Abstract T38)**
*Mohammad Ebqa'ai, Mohammad Tamimi, Andrew Kassick, Saadyah Averick, Toby L. Nelson**

10:50-11:10am **Biodegradable Aliphatic Polyesters Synthesized via Melt-Polycondensation (Abstract T39)**

*Anilkumar Yadav, Tim Dawsey, Ram K. Gupta¹**

11:10-11:30am **Effect of crystallinity on mechanical properties of poly(ethylene terephthalate) (PET) (Abstract T40)**

*Liyaqat Ali Kamran, Mohamadreza Y. Azarfam, Frank D. Blum**

Organic Chemistry (Hall 2)

Session Chair: Dr. Jeanne Bolliger

9:50-10:10am **Molecular Sculpting; a Versatile Tool for Rapid Access to Various Fluorinated Arenes via Photocatalytic Hydrodefluorination of Benzoates (Abstract T28)**

*Shivangi Kharbanda, Jimmie D. Weaver III**

10:10-10:30am **Urethanes from CO₂ and Visible Light: Putting Molecular Strain to Work (Abstract T29)**

*Timothy Schoch, Jimmie D. Weaver III**

10:30-10:50am **Domino Aza-Michael Addition-S_NAr-Heteroaromatization Route to C5-Substituted 1-Alkyl-1H-indole-3-carboxylic Esters (Abstract T30)**

*Ebenezer Ametsetor, Spencer Farthing, Richard A Bunce**

10:50-11:10am **Twisting the limits of Friedel-Crafts chemistry: Access to quaternary, diaryl, cycles through visible light photocatalysis (Abstract T31)**

*Tyler Fleske, Jimmie D. Weaver III**

11:10-11:30am **Synthesis of NOXO-BC7 (Abstract T32)**

*Osaïd Alkhamayseh, Shivangi Kharbanda, Georgia Eastham, Jimmie D. Weaver III**

Physical/Computational and Inorganic Chemistry (Conference Room 1)

Session Chair: Dr. Yihan Shao

9:50-10:10am **Theoretical Investigation of Metal Doped Gold Nano-Clusters M@Au_n (M = W, Co, and Ir) (Abstract T33)**

*Delwar Hossain**

10:10-10:30am **Hydrogen Peroxide Vapor Detection Using Low-Cost Thin Film (Abstract T34)**

*Rayhan Hossain, Allen Apblett, Nicholas F. Materer**

10:30-10:50am **Transferability of Machine Learning Potentials for Solution-Phase Reactions (Abstract T35)**

*Xiaoliang Pan, Junming Ho, Yihan Shao**

10:50-11:10am **Development of Pincer N-Heterocyclic Carbene Ligands Bearing Substituted Pyridine Linker and Their Copper (I) Complexes (Abstract T26)**

John Raincrow, Jaydon Ashley, Laleh Tahsini

11:10-11:30am **Polymer-fixed oxidation catalysts for water purification (Abstract T27)**
*Timothy J. Hubin, * Makynna R. Koper, Elisabeth Allbritton, Ashtyn McAdoo, Tuyet Hoang, Elah Alcuitas*

Chemical Education I (Conference Room 2)

Session Chair: Dr. Cammi Valdez

9:50-10:10am **Hyper Valency of Carbocations (Abstract T14)**
*A.K.Fazlur Rahman, * George Wang, Bin Wang*

10:10-10:30am **Out of the Black Box: Teaching Spectroscopy with the Wilson Analytical Open Optical Platform System (Abstract T15)**
*Allen Apblett**

10:30-10:50am **3D Printing Amino Acids as a Kinesthetic Learning Tool for Biochemistry (Abstract T16)**
*Austin Fisher, Angela Madira, Cammi Valdez**

10:50-11:10am **How do they study and does metacognition instruction make any difference in general chemistry? (Abstract T17)**
*Caroline Muteti, Carolina Zarraga, Brooke I. Jacob, Tuli M. Mwarumba, Dorothy B. Nkhata, Mwarumba Mwavita, Smita Mohanty, and Jacinta M. Mutambuki**

11:10-11:30am **Coaching Behaviors that Lead to Success in the Science Classroom (Abstract T18)**
*Christopher Jones**

11:30am-1:00pm: Lunch and Meetings

- Lunch (Cafeteria)
- Career Talk with Industry Leaders (Hall 2)
- Talk with graduate recruiters (Cafeteria)
- Section chairs meeting (Conference Room 3)

1:00-2:30pm: Poster Session (Abstracts P1-P46)

- Poster presentations: a table of presenters is shown just after the scientific program

2:30-4:30pm: Concurrent Scientific Talks

Hall 1 (Polymer II), Hall 2 (Biochemistry), Conference Room 1 (Energy and Environmental), Conference Room 2 (Chemical Education II), Conference Room 3 (Analytical)

Polymer Chemistry II (Hall 1)

Session Chair: Dr. Mitchell D. Refvik

2:30-2:50pm **Facile Mechanochemical Suzuki Polymerization for the Synthesis of Polyfluorenes (Abstract T41)**
*L. P. Tharika Nirmani, Fathima F. Pary, Toby L. Nelson **

- 2:50-3:10pm **Novel openings in utilization of animal waste for polyurethane industries (Abstract T42)**
*A.A.P.R. Perera, K.A.U. Madhushani, Felipe M. de Souza, Tim Dawsey, Ram K. Gupta**
- 3:10-3:30pm **Parameters effecting mechanical properties of composites from post-consumer polyester carpet and recycled PET resin (Abstract T43)**
*Mohamadreza Y. Azarfam, Siddhesh Chaudhari, Anuj Maheshwari, Clinton Switzer, Jay C. Hanan, Ranji Vaidyanathan, Frank D. Blum**

Biochemistry/Chemical Biology (Hall 2)

Session Chair: Dr. Gabriel Cook

- 2:30-2:50pm **Expression, Characterization, and In Vitro Glycosylation of Ectodomains from the Membrane Protein Syndecan-1 (Abstract T8)**
*Austin R. Anderson, Gabriel A. Cook**
- 2:50-3:10pm **Conjugation of Gold Nanorods with ssDNA (Abstract T9)**
*Ashley Kennedy, Dr. Nathan Green**
- 3:10-3:30pm **An Eco-Friendly method to disrupt Pheromones in *Ostrina Nubilalis*: Helping hand to farmers (Abstract T10)**
*Viswanath Nukala, Omar Al-Danoon, Shine Ayyappan, Pratikshya Paudel, Smita Mohanty**
- 3:30-3:50pm **Automated Image Analysis Tool Development for Diabetic Retinopathy (Abstract T11)**
*Anne Martin, Lauren Wilcox, Madison Whitekiller, Joshua Butcher, Dustin Baucom, Cammi Valdez**
- 3:50-4:10pm **Computational Modeling of DNA Cleavage in HNH-like Domain of I-Ppo1 (Abstract T12)**
*Richard Van, Xiaoliang Pan, Caleb Cheng Yang Gao, Yihan Shao**
- 4:10-4:30pm **Expressing, purifying and determining the structure of truncated sarcoglycan (Abstract T13)**
*James R. Bryce, Michael Harris, Gabriel Cook**

Energy and Environmental Chemistry (Conference Room 1)

Session Chair: Dr. Elijah G. Schnitzler

- 2:30-2:50pm **Instrumentation and Monitoring of Rural-Urban Gradients for Carbon Dioxide and Methane for Atmospheric Model Integration and Assimilation; Preliminary Results (Abstract T22)**
Wesley T. Honeycutt, Elizabeth Spicer, Lucas J. Livingstone, Lee Fithian, Sean M. R. Crowell
- 2:50-3:10pm **Synthesis of metal oxide nanoparticles using *Citrus reticulata* for phase and electrochemical study for energy storage application (Abstract T23)**
*Rishabh Srivastava, Shiva Bhardwaj, and Ram K. Gupta**

- 3:10-3:30pm **Reactive Uptake of Ozone in the Indoor Environment: Commercial Dyes and Respiratory Aerosol (Abstract T24)**
*Habeeb H. Al-Mashala, Katrina L. Betz, Christian Escritt, E. Addie Coody, Alison M. Boone, and Elijah G. Schnitzler**
- 3:30-3:50pm **Hydrothermal-assisted bi-metallic MOF for hydrogen evolution and energy storage applications (Abstract T25)**
*Shiva Bhardwaj, Rishabh Srivastava, Teddy Mageto, Sudhakar Reddy, Ram Gupta**

Chemical Education (Conference Room 2)

Session Chair: Dr. Jacinta M. Mutambuki

- 2:30-2:50pm **Making them see the relevance: the impact of integrating real-world contexts and application cards activities on students' learning outcomes in General Chemistry I lecture course (Abstract T19)**
*S.M. Ifat Hossain Sristy, Yolanda Vasquez, Jacinta M. Mutambuki**
- 2:50-3:10pm **Using survey data to increase student engagement and retention in the organic chemistry classroom (Abstract T20)**
*Donna J. Nelson**
- 3:10-3:30pm **Voices of chemistry role models versus metacognition instruction: How do they impact learning outcomes in General Chemistry courses? (Abstract T21)**
*Shanmugam Puvanendran, Tracy Kerr, and Jacinta M. Mutambuki**

Analytical Chemistry (Conference Room 3)

Session Chair: Dr. Gabriel LeBlanc

- 2:30-2:50pm **Authentication of Edible Oils Using an Infrared Spectral Library and Digital Sample Sets (Abstract T2)**
*Collin G. White, Isio Sota Uba, Karl Booksh, and Barry K. Lavine**
- 2:50-3:10pm **Application of Ultramicrotomy and Infrared Imaging to the Forensic Examination of Automotive Paint (Abstract T3)**
*Elizabeth Donkor, Haoran Zhong, Kaushalya Sharma Dahal, George Affadu, Barry K. Lavine**
- 3:10-3:30pm **3D Printing to Address Challenges in Electrochemistry (Abstract T4)**
*Gabriel LeBlanc**
- 3:30-3:50pm **Raman Spectroscopy to Enhance Investigative Lead Information in Automotive Clearcoats (Abstract T5)**
*Haoran Zhong, George P. Affadu-Danful, Kaushalya Sharma Dahal, Kaan Kalkan, Linqi Zhong, Barry K. Lavine**
- 3:50-4:10pm **Coupling Sensitive Surface Plasmon Signals with a Colorimetric Sensor Reaction: Urine and Serum Matrices (Abstract T6)**
*Zhuo Wang, Zia Syed, Zainab H Al Mubarak, Lucy Lehoczky, Cassandra Rodenbaugh, and Sadagopan Krishnan**

4:10-4:30pm **Kinetic and Thermodynamic Characterization of Colloidal Polymers of N-isopropylacrylamide and Alkyl Acrylic Acids for Optical pH Sensing (Abstract T7)**
*Thomas Moulton, David Bruce, and Barry K. Lavine**

4:40-4:50pm: Concluding Remarks & Meeting Adjournment

Dr. Raj Kailasam (General Co-Chair, 65th Pentasectional Organizing Committee)

Poster Presenter List

| Division | | Presenter | Title | Institute |
|------------------------|-----|------------------------------|--|------------------|
| Analytical | P1 | Audra Crisp | Spectrophotometric Determination of Metal Complex pKas | SWOSU |
| Analytical | P2 | Meena Seshadri | Optimization of Higher-Energy Collisional Dissociation Fragmentation Energy for Intact Protein-level Tandem Mass Tag Labeling | OU |
| Biochemistry | P3 | Abhijtkumar Jayasekar | The Effect of HK2 on Lymphatic Vessel Development | Ok Med Res Found |
| Biochemistry | P4 | Charli Woessner | Synthesis of Gold Nanoparticles | NSU |
| Biochemistry | P5 | Damodar Pai | Quality Control Systems with HLA DP | OSSM |
| Biochemistry | P6 | Eon Lim | Cloning of Human cDNA into the Lentiviral Vector | OSSM |
| Biochemistry | P7 | Jhawn Saul | Hydroxamic Acid Compounds for Inhibition of Metallo- β -Lactamase from <i>Bacillus anthracis</i> | NSU |
| Biochemistry | P8 | Jonas G. Ewusi | Expression, Purification, and Glycosylation of γ -sarcoglycan | OSU |
| Biochemistry | P9 | Maia Gugello | Inhibition of Metallo-beta-lactamase from <i>Bacillus anthracis</i> by Hydroxybenzoic Acid | NSU |
| Biochemistry | P10 | Natalie O'Guin | Synthesizing Aspirin Analogs to Inhibit HDAC1 | NSU |
| Biochemistry | P11 | Ovea Kaushik, Meena Seshadri | Mechanisms of Resveratrol in Inhibiting Cancer | OSSM |
| Biochemistry | P12 | Pratikshya Paudel | An Eco-Friendly method to disrupt Pheromones in <i>Ostrina Nubilalis</i> : Helping hand to farmers | OSU |
| Biochemistry | P13 | Rachel Galfo | Conjugating Modified DNA to Thiolated Silica Nanoparticles Towards Nanoparticle Self-Assembly | NSU |
| Biochemistry | P14 | Sarah Faubion | Inhibition of New Delhi Metallo-Beta-lactamase-1 (NDM-1) by Benzamide Derivatives | NSU |
| Biochemistry | P15 | Tiwalola Ogunleye | Recombinant expression and purification of membrane proteins; T-cell receptor alpha (TCR α) and Transmembrane serine protease II (TMPRSS2) | OSU |
| Biochemistry | P16 | Trent Brown | Inhibition of Bal2 by Hydroxamate-containing Compounds | NSU |
| Chemical Education | P17 | Charles Crittell | Molecules of Nature: A Summer Academy | ECU |
| Chemical Education | P18 | Farouk Awudu | The Impact of Authentic Research-Based Experiences on Students' Learning Outcomes in General Chemistry I Laboratory Course | OSU |
| Energy and Environment | P19 | Katrina L. Betz | Physical and Optical Properties of Biomass Burning Organic Aerosol from Eastern Red | OSU |

| | | | | |
|--------------------------|-----|------------------------------------|---|---------|
| | | | Cedar: Hygroscopicity, Absorbance, and Polarity | |
| Energy and Environmental | P20 | Ciara Kelley | Sorbent to Fertilizer Technology for Environmentally Friendly Water Treatment | OSU |
| Energy and Environmental | P21 | Colton T. Calvert | Biomass Burning Organic Aerosol from Summer and Winter Tallgrasses on the Great Plains: Absorbance, Hygroscopicity, and the Role of Charge-Transfer Complexes | OSU |
| Energy and Environmental | P22 | Natalia Araujo da Silva | Mechanochemical Synthesis of Cyclodextrin-Molybdenum Oxide Nanocomposites | Cameron |
| Energy and Environmental | P23 | Patrick Kitzel | Mg ²⁺ /Al ³⁺ Layered Double Hydroxide Synthesis for Phosphate and Nitrate Removal | OSU |
| Energy and Environmental | P24 | Sithumi M. Liyanage | Formation of Hydrogen Peroxide in Commercial Aerosol Generators: Detection, Quantification, and Implications | OSU |
| Inorganic | P25 | Christian Hunt | Synthesis, Characterization and Photoluminescent Studies of Two and Three-Coordinate Cu(I) Complexes bearing Diaminocarbene Ligands | OSU |
| Inorganic | P26 | Emmy Huang | Fourier-Transform Infrared Spectroscopy Study of Asphalt Aging and Its Effect on Chemical Composition | OSSM |
| Inorganic | P27 | Matthew Clark | : Investigation of the Photophysical Effects of Cysteamine as an Aqueous-phase Ligand for CuInS ₂ /ZnS Core-Shell Quantum Dots | NSU |
| Inorganic | P28 | Nima Noei | Synthesis and characterization of tri-dentate quinoline-based OCN ligands and their complexes | OSU |
| Inorganic | P29 | Sarvesh Ramakrishnan | Synthesis, X-ray, and Theoretical Structural Analysis of A Binuclear Manganese Tricarbonyl Thionicotinic Acid Complex | OSSM |
| Inorganic | P30 | Tsitsi Kapfunde | Nucleophilic attack at the bound NO of cationic group 8 nitrosyl porphyrins | OU |
| Organic | P31 | Allison P. Hussin | Electro-organic synthesis using 3D-printed electrodes | TU |
| Organic | P32 | Catrina Aguirre | Optimization of the Synthesis of Substituted 1,2,4-Triazoles | OSU |
| Organic | P33 | Georgia Eastham | Adaptation of strain loadable alkenes for biological uses | OSU |
| Organic | P34 | Justin Childress, Audrey Jergensen | Amino Acid Exchange in Ni(II) Complexes of Glycine | SWOSU |
| Organic | P35 | Kaitlin Ashcraft | Hantzsch Amides for the Selective Reduction of Michael Acceptors | OSU |
| Organic | P36 | Nathan Herndon | Broadening the Boundaries of Friedel-Crafts: Access to 1,1-diarylcyclohexyl motifs through visible light photocatalysis | OSU |
| Organic | P37 | Rachel Crittall | Access to Tricyclic Heteroarenes by an Iodine-promoted Cyclization Reaction | OSU |

| | | | | |
|------------------------|-----|--|---|---------|
| Organic | P38 | Rachel Gerick | Efforts Toward Synthesis of Sideromycins with Catenulobactin B to Improve Antibiotic Penetration into Gram-Negative Bacteria | ORU |
| Organic | P39 | Rehema Nakiwala | Access to substituted tricyclic heteroarenes by an oxidative cyclization reaction | OSU |
| Organic | P40 | Roshini Hanumanthu | Lutidine enabled Photocatalytic Giese type reactions of alkyl/aryl halides | OSU |
| Organic | P41 | Tori I. Cole | 3D Printed Electrodes and Devices for Electro-Organic Synthesis | TU |
| Physical/Computational | P42 | Daniel Kim, Jason Cousineau | Probing electronic and hydrodynamic properties of fluorescent probe molecules in reverse micellar environment | Cameron |
| Physical/Computational | P43 | Hannah Spoon | Photophysical and hydrodynamic properties of Alexa Fluoro (AF) 647 dyes in confined reverse micellar environment in presence of Graphene Oxide nanoparticle | Cameron |
| Physical/Computational | P44 | Sang Lee, Kap H, Sang, Gary Ritzhaupt, Catherine Klehm, Prathibha Desman | 19 K Argon Matrix Isolated 5-Fluoro-2'-Deoxyuridine Analyzed by Vibrational Spectroscopy and Supercomputer Calculations using GAMESS | ORU |
| Physical/Computational | P45 | Wesley A. Horn, Alberto Corredor | Study of Electronic Properties of Pi-electron Systems Containing Silicon-Silicon Double Bonds Using Density Functional Theory | OSSM |
| Physical/Computational | P46 | Zackory D. Boiselle, Chang-Yang Yang, Hannah N. Smith, Lois Ablin, Gary Ritzhaupt, Catherine Klehm | FTIR Spectroscopy of Ethyl 6-Methyl-4-Phenyl-2-Sulfanylidene-1,2,3,4-Tetrahydropyrimidine-5-Carboxylate Matrix Isolated in 18 K Frozen Argon | ORU |

T1: Keynote Talk by Mitchell D. Refvik

Developing Circular Solutions in the Petrochemicals Industry

Mitchell D. Refvik

Senior Manager Polyolefin Catalysis
Chevron Phillips Chemical Company LP

Since the development of the polymers industry, plastics have become a widely accepted packaging option worldwide for good reason - these materials are known their high strength, light weight, extraordinary flexibility, low energy usage and low toxicity. But these same materials that offer so many societal advantages are also under increasing environmental scrutiny due largely to gaps in the infrastructure required to handle post use materials.

Industry is engaged in an unprecedented effort to create and deploy sustainable circular approaches that address end of life innovations designed to reclaim valuable hydrocarbon resources and return them to commerce – that is, developing a circular economy.

In this seminar, we will explore the innovations that have made synthetic polymers the material of choice for so many applications, the drivers behind the growth of this industry, the challenges we face, solutions under development and the collaborative efforts needed to responsibly repurpose post use plastics to circular solutions that meet societal needs.

Oral Presentation Abstracts

T2: Authentication of Edible Oils Using an Infrared Spectral Library and Digital Sample Sets

Collin G. White¹, Isio Sota Uba¹, Karl Booksh², and Barry K. Lavine^{1*}

¹*Department of Chemistry, Oklahoma State University, Stillwater, OK 74078*

²*Department of Chemistry & Biochemistry, University of Delaware, Newark, DE 19716*

Email: collin.white@okstate.edu (Presenter)

A potential method to determine whether two varieties of edible oils can be differentiated by Fourier transform infrared (FTIR) spectroscopy is proposed using digitally generated data of adulterated edible oils from an infrared (IR) spectral library. The first step is the evaluation of digitally blended data sets. Specifically, IR spectra of adulterated edible oils are computed from digitally blending experimental data of the IR spectra of an edible oil and the corresponding adulterant using the appropriate mixing coefficients to achieve the desired level of adulteration. To determine whether two edible oils can be differentiated by FTIR spectroscopy, pure IR spectra of the two edible oils are compared to IR spectra of two edible oils digitally mixed using pattern recognition techniques to solve a ternary classification problem. If the IR spectra of the two edible oils and their binary mixtures are differentiable, then differences between the IR spectra of these two edible oils are of sufficient magnitude to ensure that a reliable classification by FTIR spectroscopy can be obtained. Using this approach, the feasibility of authenticating edible oils such as extra virgin olive oil (EVOO) directly from library spectra is demonstrated. For this study, both digital and experimental data are combined to generate training and validation data sets to assess detection limits in FTIR spectroscopy for the adulterants.

T3: Application of Ultramicrotomy and Infrared Imaging to the Forensic Examination of Automotive Paint

Elizabeth Donkor, Haoran Zhong¹, Kaushalya Sharma Dahal¹, George Affadu¹, Barry K. Lavine^{1*}

¹*Department of Chemistry, Oklahoma State University, Stillwater, OK 74078*

Email: elidonk@okstate.edu

In a previously published study, Lavine and coworkers demonstrated that infrared spectra from all layers in an intact multilayered OEM paint chip can be collected in a single analysis by scanning across each layer of a cross-sectioned paint chip using an FTIR imaging microscope. Applying alternating least squares to the spectral data, the infrared spectrum of each layer of an OEM paint chip can be successfully reconstructed from a line map of its spectral image. To further develop this imaging technique for automotive paint analysis, the capability to analyze “small” paint chips and higher spatial resolution will be leveraged with the current imaging method. Specifically, cross sectioning will be performed using an ultramicrotome which does not require epoxy or any other embedding media, thereby simplifying the analysis and allowing small paint chips to be cross sectioned and accessible for spectral imaging. Furthermore, a new type of infrared microscope that utilizes a beam with a smaller spot size to interrogate the cross sectioned paint sample will be employed. The proposed methodology would not only eliminate the need to analyze each paint layer separately but also ensure that an infrared spectrum of each layer is pure and not a mixture of two layers which can occur as a result of sampling too close to the boundary between adjacent layers when using a scalpel to separate adjacent layers. Not having a “pure” spectrum of each layer prevents a meaningful comparison between each paint layer, or in the situation of searching an automotive paint database, prevents the scientist from developing an accurate hit list of suspected vehicles. Furthermore, the advantages inherent in two very different approaches to automotive paint analysis (Royal Canadian Mounted Police versus European Forensic Laboratories) will be realized with the proposed imaging method. Using a new sample preparation technique and an IR microscope with higher spatial resolution, a forensic paint examiner will be able to obtain both high quality IR spectra and visual color information from paint fragments that are smaller than what is practical to handle by hand-sectioning.

T4: 3D Printing to Address Challenges in Electrochemistry

Gabriel LeBlanc*

The University of Tulsa, Department of Chemistry and Biochemistry

Email: Gabriel-leblanc@utulsa.edu

3D printing is a rapid prototyping technique that allows for unique equipment to be quickly developed for a wide variety of applications. Due to the ability to quickly share the digital designs and the availability of 3D printing hardware, the application of 3D printing for scientific research has grown rapidly. Because of the unique geometries involved in many electrochemical devices and experiments, there are a variety of ways that 3D printing can be used to accelerate progress in the field. In this presentation we will discuss some of the recent advances in the application of 3D printing in electrochemistry, particularly those involving fuse-filament fabrication methods.

T5: Raman Spectroscopy to Enhance Investigative Lead Information in Automotive Clearcoats

Haoran Zhong¹, George P. Affadu-Danful¹, Kaushalya Sharma Dahal¹, Kaan Kalkan², Linqi Zhong²,
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Modern automotive paints typically use thinner undercoat and color coat layers protected by a thicker clear coat layer. All too often, the clear coat is the only layer of automotive paint left at the crime scene of a vehicle related fatality such as a hit-and-run where injury or death to a pedestrian has occurred. Current approaches used by Paint Data Query (PDQ), the largest forensic automotive paint database in the world, to identify clear coats have been unsuccessful because the infrared (IR) spectra of clear coats are too similar to generate accurate hit lists by searching clear coat IR spectra alone. Recently published studies of pattern recognition methods applied to IR spectra of clear coats have shown that information about the line and model of the vehicle can be obtained from these spectra. To further enhance the general discrimination power of automotive clear coats, Raman spectroscopy and pattern recognition techniques will be investigated as a potentially better solution to the problem of extracting investigative lead information from clear coats. The general discrimination power of Raman for automotive paint comparisons involving 118 General Motors clear coat paint samples (spanning six assembly plants for the production years 2000-2006) will be compared to previous results obtained using IR spectroscopy. The spectral region from 1802 – 697 cm^{-1} was found to be supportive in the discrimination of these six General Motors assembly plants using Raman spectroscopy. By comparison, only one of the six vehicle assembly plants (Moraine) could be differentiated from the other five assembly using IR spectroscopy and pattern recognition methods. The results of this study suggest that Raman spectroscopy in combination with pattern recognition methods offers distinct advantages over IR spectroscopy for the identification and discrimination of automotive clear coats.

T6: Coupling Sensitive Surface Plasmon Signals with a Colorimetric Sensor Reaction: Urine and Serum Matrices

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Formaldehyde is an environmental pollutant. Detection of low harmful exposure levels of formaldehyde indoors and that of disease-relevant ultra-low ppb concentrations is challenging due to the small size of this molecule, which does not yield enough signal changes in sensors at low concentrations in comparison to large biomolecules (e.g., DNA, proteins, and antibodies). Hence, various surfaces, material designs, and analytical strategies have constantly been developed to achieve low detection limits of formaldehyde. Herein, we demonstrate a sensing strategy of coupling surface plasmon resonance imaging with colorimetric formaldehyde detection using the Purpald reagent (4-amino-3-hydrazino-5-mercapto-1,2,4-triazole) to enable an ultra-low detection limit (86 parts per trillion) compared with 12 ppb detection limit of traditional UV-visible method. Formaldehyde recovery in spiked 50-times diluted serum was 92%. In urine, due to the observed interference from urea, the sample recovery was relatively lower (67%). High selectivity was observed in comparison experiments using one ppm of various analytes in buffer solution. Thus, the concept of hyphenating sensitive surface plasmon transduction principle with colorimetric reactions has the potential to amplify analyte detection signals suitable for health and environmental applications.

T7: Kinetic and Thermodynamic Characterization of Colloidal Polymers of N-isopropylacrylamide and Alkyl Acrylic Acids for Optical pH Sensing

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Copolymers of N-isopropylacrylamide (NIPA) and alkyl acrylic acids that swell and shrink in response to pH were prepared by dispersion polymerization at 35°C using N-isopropylacrylamide (transduction monomer), methylenebisacrylamide (crosslinker), 2-dimethoxy-2-phenyl-acetophenone (initiator), *N*-tert-butylacrylamide (transition temperature modifier), and acrylic acid, methacrylic acid, ethacrylic acid or propacrylic acid (functional comonomer). The diameter of the microspheres was between 0.5 μm and 1.0 μm. These microspheres were cast into hydrogel membranes prepared by mixing the pH sensitive swellable polymer particles with aqueous polyvinyl alcohol (PVA) solutions followed by crosslinking with glutaric dialdehyde for use as pH sensors. Large changes in the turbidity of the PVA membrane were observed as the pH of the buffer solution in contact with the membrane was varied. Changes in turbidity were monitored using a Cary 6000 UV-visible absorbance spectrometer. Polymer swelling was reversible for many of the NIPA copolymers. The buffer capacity, pH and temperature of the solution in contact with the membrane were varied to provide an in-depth pH profile of each copolymer. A unique aspect of this study was the investigation of the response of the NIPA based polymers to changes in the pH of the solution in contact with the membrane at low buffer capacities (0.5 mM). The rapid response rate and the reversibility of polymer swelling even at low buffer capacities suggest that NIPA based copolymers can be coupled to an optical fiber for pH sensing. We envision using these polymers to monitor rising acidity levels in the ocean due to water that has become enriched in carbon dioxide, endangering shell building organisms by reducing the amount of carbonate available in the water for them.

T8: Expression, Characterization, and In Vitro Glycosylation of Ectodomains from the Membrane Protein Syndecan-1

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Membrane proteins are a key component of numerous biological processes such as signal transduction, transportation, and various cell-cell interactions. Nearly one-third of all genes encode for membrane proteins and around one-half of all drug targets are membrane proteins. Despite the significance of these proteins, a relatively small amount of membrane protein structures have been determined. Membrane proteins are difficult to express in high quantities and contain highly hydrophobic domains that generally require solubilization strategies using detergents or lipids. Post-translational modifications further diversify these proteins. Many membrane proteins are glycoproteins with one or more sugar attachment sites. Glycosylation, like other types of post-translational protein modifications, can have a profound effect on the structure and function of these proteins. Syndecan-1 (SDC-1), an integral membrane glycoprotein, is involved in the body's innate immune response system. When cells are under stress due to infection or trauma, the ectodomains of SDC-1 are cleaved and released into the bloodstream as a way to induce formation of a chemokine gradient that subsequently recruits leukocytes to the affected area. The shedding of SDC-1 has been shown to become upregulated in a multitude of cancer types. This protein is normally highly glycosylated in nature with one N-linked glycosylation site and five O-linked glycosylation sites. While many important biological functions of SDC-1 have been identified, its structure and specific interactions have not been elucidated. We have successfully expressed, purified and glycosylated SDC-1 using in vitro glycosylation in order to study how glycosylation affects protein structure, dynamic

T9: Conjugation of Gold Nanorods with ssDNA

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Gold nanorods (GNRs) are inert materials that can serve a multitude of practical applications in complex materials assemblies. In this work, methods will be explored for the establishment of DNA conjugated GNRs. Once the GNR surface is successfully functionalized with single-stranded DNA (ssDNA), these nanorods will be useful both individually and when combined. Specifically, when combined with a corresponding DNA-based scaffold, these conjugated GNRs can be used to form an aggregate that will serve as a model for self-assembly. One of the most common issues when working with nanoparticles is a lack of versatile self-assembly methods. This project aims to create a DNA based scaffolding system to address that lack. The GNRs in this work were synthesized using a two-step, silver-assisted, seeded growth. DNA-nanoparticle conjugates were produced via surface functionalization and subsequent exposure to ssDNA in selective coupling reactions. In an agarose gel, two different sets of conjugated GNR samples pulled through the gel, indicating successful conjugation. Nonconjugated GNRs did not pull through the gel. A protocol was established for successfully and consistently creating DNA-conjugated GNRs.

T10: An Eco-Friendly method to disrupt Pheromones in *Ostrina Nubilalis* : Helping hand to farmers.

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European corn borer (ECB) *Ostrinia nubilalis* (Onub), is a very serious pest of corn, sweet corn, and other crops. ECB accounts for 5.5 to 8.5 million ton of corn loss in an average year in Europe and other countries. ECB was introduced to United States in the 1900s. This pest accounts for 20% of yield loss in North America with damages estimated to exceed US \$1 billion annually. Pesticides and insecticides used to control these pests cause harmful effects in the environment. Moreover, pests show resistance to it. Thus, there is an urgent need for an alternate method for pest control. Mating in lepidopteran moths such as *Ostrinia nubilalis* is initiated with the detection of female-secreted pheromones by the males. The pheromone binding proteins (PBPs) present in the male moth antenna play a critical role in pheromone detection. Of the five PBPs identified in *Ostrinia nubilalis*, OnubPBP2 and OnubPBP3 have male-biased expression. An alternate approach for pest control is to target the mating process by intervening in the pheromone detection system of the male moth. Structure-function study of the OnubPBP2 is critical to interfere in the pheromone detection system of this invasive insect pest in a species-specific and environmentally friendly manner. To achieve this goal, we have cloned, expressed, purified, and investigated the recombinant OnubPBP2 through biophysical characterization. We have determined the high-resolution 3-dimensional structure of OnubPBP2 by NMR spectroscopy.

T11: Automated Image Analysis Tool Development for Diabetic Retinopathy

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Diabetic retinopathy, a complication of diabetes that degrades the retinal vasculature, is the leading cause of blindness in working adults. Diabetic retinopathy is treated in its later stages, when the retina forms new, leaky blood vessels that cause visual impairment. Although the later stages of diabetic retinopathy are most detectable, one of the earliest stages of diabetic retinopathy is the dropout of retinal pericytes, which line the outer layer of retinal capillaries. In normal retinal vasculature, pericytes exist in a 1:1 ratio with endothelial cells, which are cells that compose the inner layer of retinal capillaries. In retinal vasculature affected by diabetes, however, the ratio of pericytes to endothelial cells shifts from 1:1 to 1:4. Identifying this pericyte dropout is essential to detecting early stages of diabetic retinopathy, but analysis of retinal vasculature images is time-consuming and tedious, especially with mouse retinal imaging.

In order to detect and evaluate the impact of diabetic pericyte dropout objectively and more quickly, the Valdez Lab has created an automated image analysis program. The images utilized for automated analysis are mouse retinal vasculature, isolated via elastase digest and imaged using brightfield microscopy. A pipeline was developed in CellProfiler, a free-to-use image analysis program, to trace and identify both endothelial cells and pericytes in mouse retinal microvasculature. Our pipeline accounts for cells that are obscured by image borders, and thus removes these cells that cannot be properly identified from analysis. Since blood vessels larger than capillaries contain smooth muscle cells instead of true pericytes, cells associated with larger vessels are eliminated by a separate algorithm developed by our group. Once established, the automated image analyses are compared to manual image analyses. Identifying pericytes and endothelial cells via automated image analysis quantifies the number of both types of cells without bias and reduces analysis time by 20-fold. The development of this new automated image analysis tool sets the foundation for detecting pericyte dropout in diabetic retinopathy.

T12: Computational Modeling of DNA Cleavage in HNH-like Domain of I-Ppo1

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Gene therapy can treat diverse clinical indications and tissue targets by utilizing nucleases to target specific regions of DNA. To date, CRISPR-Cas9 remains as one of many popular enzymes to induce genetic modification, but the translation to human clinical trials has been limited. Those shortcomings can include DNA/RNA specificity, therapeutic delivery, and/or toxicity which highlights the need for development of safer gene editing technologies. Fundamentally, a greater understanding of how Cas9 cleaves DNA would help facilitate this, however, the precise mechanism has not been well understood.

In recent years, Molecular Dynamics (MD) and Quantum Mechanics/Molecular Mechanics (QM/MM) simulations have become an integral part of the protein engineering workflow. These virtual experiments can provide insight into how amino acid mutations can affect DNA cleavage, DNA binding, or structural rearrangements. For this study, we performed MD and QM/MM simulations on the homing endonuclease, I-Ppo1. This enzyme contains an HNH-like domain analogous to the target strand DNA cleavage domain of Cas9. Unlike the CRISPR-Cas systems, homing endonucleases do not require a guide-RNA to cleave DNA, rather, they contain large DNA interfaces allowing for up to thirty DNA base pair recognition. A key feature which has made meganucleases vital to our current understanding genetic engineering. From our calculations, we found that H98 can deprotonated a nearby water thereby initiating the nucleophilic attack on DNA. This resulted in a free energy barrier of $\sim 23.8 \pm 0.2$ kcal/mol agreeing well with the experimentally observed k_{cat} of 0.0023 min^{-1} in wild-type I-Ppo1.

The work highlighted in this talk not only provides the first free energy profile of I-Ppo1 H98-mediated DNA cleavage, but a computational approach to the study of other HNH containing enzymes such as CRISPR-Cas9.

T13: Expressing, purifying and determining the structure of truncated sarcoglycan

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Sarcoglycans are transmembrane proteins that play an important role in the dystrophin complex. by maintaining the integrity of the muscle fiber sarcolemma by connecting the cytoskeleton of the muscle fiber to the extracellular matrix. Mutations of the gene that encodes the sarcoglycan protein can result in the development of muscular dystrophies. The truncated form of the γ -sarcoglycan has a small intracellular domain, one transmembrane domain and a shortened extracellular sequence. The extracellular structure contains a single glycosylation site that is believed to play an important role in the structure of the protein. We have recombinantly overexpressed the truncated protein in *e. coli* so that isotopically labeled protein can be purified to look at the structure and dynamics of the protein using NMR spectroscopy. We also plan to use *in vitro* glycosylation to look at the affect on structure, dynamics and interactions of γ -sarcoglyca. We hope that by studying this protein we can determine the structure of the protein as well as the protein-protein interactions of this protein in an effort to develop treatments for muscular dystrophy.

T14: Hyper Valency of Carbocations

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The vituperative decades long debate between classical and non-classical depiction of 2-norbornyl cation has recently been resolved by the X-ray crystallographic proof of the bridged non classical geometry of the solvated $[\text{C}_7\text{H}_{11}]^+ \{\text{Al}_6\text{Br}_7\}\text{CH}_2\text{Br}_2$ salt. The hyper valency of carbon beyond four was formulated to six in 2017 by Mortiz and Seppelt by confirming the pentagonal pyramidal framework in dicationic hexamethyl benzene by reporting its X-ray crystal structure. This presentation will discuss how a 17-year-old high Schooler in Oklahoma proposed a heptavalent tri cationic carbon in 2018 to become a part of the story of the very elusive carbocation.

T15: Out of the Black Box: Teaching Spectroscopy with the Wilson Analytical Open Optical Platform System

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Modern spectrometers in teaching laboratories tend to be closed systems where a sample is placed in a sample holder isolated from the optical components so that the actual workings of the instrument remain opaque. The Wilson Analytical Open Optical Platform System circumvents this restriction and has significant potential to revolutionize the teaching of spectroscopy and instrumental analysis both in introductory chemistry and upper level courses. The open architecture of the system can be used to teach students how ultraviolet-visible and fluorescence spectroscopy systems are configured and how they work. This includes considerations of how absorbance and fluorescence systems are configured differently, the influence of light source intensity on experimental measurements, the influence of stray light, and signal to noise determinations. In particular, the inherent superiority of fluorescence over light sorption measurements for the determination of low concentrations of analytes is readily demonstrated on this platform. Furthermore, an available solid-state accessory makes measuring spectra of solids very easy and is a boon to laboratory experiments that produce insoluble colored compounds or where one wishes to avoid extraction procedures and the expense and disposal of organic solvents. For example, experiments can be performed where chlorophyll is analyzed by absorption spectroscopy using extracts from spinach or chlorophyll-containing gum. Alternatively, the extracts can be analyzed by fluorescence spectroscopy or the gum and spinach leaves can be analyzed directly using the solid-state accessory.

T16: 3D Printing Amino Acids as a Kinesthetic Learning Tool for Biochemistry

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Proteins are at the center of course content for Biochemistry. Beginning with primary amino acid sequence, moving into protein secondary, tertiary, and quaternary structures, and then ultimately exploring protein function, Biochemistry investigates proteins in depth throughout the semester. Amino acids are the building blocks of proteins, and therefore foundational and core to the topics taught in undergraduate Biochemistry courses. To have a better understanding of the role amino acids play in proteins and biological systems more broadly, it is important for Biochemistry students to become familiar with amino acids and their structures.

In this project, we aim to determine if the use of a kinesthetic learning tool will increase short- and long-term undergraduate student knowledge retention of amino acids and their structures. The treatment group received a set of 3D printed amino acids to study from and was assigned an amino acid to create using Blender, an open-source 3D modeling software. Quantitative data was collected in the following formats: pre-assessment, quiz, test, and final exam. The treatment group completed an additional quantitative survey online and qualitative interview in person on their experience with designing and studying from 3D printed amino acids. Undergraduate students overwhelmingly reported that designing a 3D amino acid provided a sense of accomplishment, was satisfying to complete, and added value to their experience in Biochemistry. Short-term structural knowledge retention was improved in the treatment group, as determined by their quiz and exam scores. This was further acknowledged by the undergraduate student participants who indicated that designing a 3D amino acid and using the set of 3D amino acids improved their knowledge of amino acid structure. A majority of students indicated they would recommend this assignment to future students. Through this work, we have shown that incorporating 3D printing as a kinesthetic learning tool in Biochemistry not only improves short-term undergraduate student knowledge retention of amino acid structure, but also provides an engaging mechanism for students to interact with content that adds value to their learning experience.

T17: How do they study and does metacognition instruction make any difference in general chemistry?

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Teaching first-year college students metacognitive strategies early in their study programs can help them adopt and sustain effective study strategies throughout their college training, and boost their chances of matriculation to STEM programs. While a handful of studies have looked at study strategies among students in the general chemistry course as well as the impact of metacognitive activities on student achievement scores in chemistry, very few studies, if any, have examined the influence of explicit teaching of metacognition on students' study strategies. Training students on metacognition, "thinking about thinking" can enhance their knowledge of effective study strategies, when to use them, and why, as well as self-regulated learning. Using open-ended questionnaires, we investigated general chemistry students' perceived study strategies that they used before a 50-minute metacognition lesson, immediate gains on study strategies after the metacognitive lesson, reported adoption of specific metacognitive strategies over the course of a semester, and the impact on performance in the final exam. In addition, the reported transfer of the metacognitive strategies to other STEM courses was investigated. Findings showed that rote memorization was more frequently reported over higher-order study strategies prior to the metacognition training, but there was a shift to adopting higher-order study strategies including metacognitive strategies after the metacognition training. Moreover, more AB letter grades were associated with students who reported a positive impact on the instruction, and 55% of the participants reported the transfer of metacognitive strategies to other STEM courses. Detailed findings and implications for practice will be presented.

T18: Coaching Behaviors that Lead to Success in the Science Classroom

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Chemistry instructors want to see their students consistently get the right answers on questions to demonstrate mastery of the topics being assessed. Success is showing you can get the correct answer. They often celebrate these successes as a way to reinforce their students' efforts. While this is not a bad strategy, it places encouragement at the end of the process. This author seeks to describe a methodology which encourages or coaches the behaviors students can take as they are moving along the path to success. This presentation will examine the analogy of a distance runner and the training needed to improve. Metacognition, thinking about thinking, will be defined and applied to the learning process. An example of how to coach behaviors that lead to success for unit conversions will be detailed.

T19: Making them see the relevance: the impact of integrating real-world contexts and application cards activities on students' learning outcomes in General Chemistry I lecture course.

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Past studies have reported attrition in STEM disciplines partly due to the lack of content relevance. Unfortunately, content relevance has been integrated into the chemistry laboratory in terms of modules in which experiments are designed to reflect real-world contexts; thus, the benefits of context-based laboratory learning are somewhat understood. Although attempts to integrate real-world contexts in chemistry for non-STEM majors have shown accrued benefits, studies investigating the impact of the integration of real-world contexts into postsecondary chemistry lecture courses for STEM majors have been overlooked. To attract and retain students in STEM programs, general chemistry lecture courses can be revamped to enhance relevance to students. This study is the first to our knowledge to investigate the impact of integrating real-world contexts and application card activities—student-generated responses on the relevance of the learned chemistry concepts to their daily experiences, into the chemistry lectures on students' perceived relevance of chemistry. This study was guided by three research questions. (1) What is the impact of integrating real-world contexts into the General Chemistry I lecture course on students' perceptions of chemistry? (2) How do the embedded real-world contexts in chemistry problem sets and application card activities impact students' learning experiences in the General Chemistry I course? (3) Are there any differences in performance between students who are exposed to real-world contexts and their counterparts who are not in the General Chemistry I lecture course? A mixed-methods approach was employed. Preliminary findings showed improved perceptions of chemistry relevance to students exposed to real-world contexts and application card activities than their counterparts who did not do these interventions. Detailed data analysis and results will be discussed.

T20: Using survey data to increase student engagement and retention in the organic chemistry classroom

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Surveys combined with direct student input are used to explore students' attitudes and opinions. Together, these yield data which can be used to indicate the success of teaching methodologies for increasing student retention. This process can be used to determine suitability and acceptability of new educational practices or combinations of those practices. The implementation of this will be presented. The following will be identified and discussed: the activities which have been combined and used, the activities which led to their identification and combination, and measurement of student impact via mindset surveys.

T21: Voices of chemistry role models versus metacognition instruction: How do they impact learning outcomes in General Chemistry courses?

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Chemistry classrooms are becoming more diverse than ever. However, attrition continues to be a national concern in STEM courses, including the gateway chemistry courses, especially for historically excluded groups in STEM. Thus, there is a critical need for instructional innovations and adaptations to facilitate equitable learning outcomes for all students. Creating inclusive learning environments and training students on effective study strategies can increase their performance and sense of belonging in chemistry and STEM programs. Using a quasi-experimental design, we investigated the impact of metacognition instruction versus the integration of voices of marginalized faculty and student role models in chemistry on performance and sense of belonging in General Chemistry I and II courses as well as STEM programs. Current preliminary results show that although the differences in performance scores between students exposed to metacognitive strategies versus those exposed to the voices of role models were not statistically significant ($p > 0.05$) in both courses, students exposed to metacognitive strategies in General Chemistry I performed slightly better than those exposed to the voices of role models. However, the role models group reported more sense of belonging in the two General Chemistry courses compared to the metacognition group. Detailed data collection, results, and implications for practice will be discussed.

T22: Instrumentation and Monitoring of Rural-Urban Gradients for Carbon Dioxide and Methane for Atmospheric Model Integration and Assimilation; Preliminary Results

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In preparation for the 2024 launch target of the NASA's Geostationary Carbon Cycle Observatory (GeoCarb), the science team for the project is preparing terrestrial instrumentation for calibration and validation work. The GeoCarb team has deployed similar optical total column instruments variously co-located with terrestrial gas sensing, uncrewed aerial systems (UAS) mounted gas sensing, and meteorological instrumentation. Additionally, the team incorporated datastreams from atmospheric models such as the weather research and forecasting greenhouse gas (WRF-GHG) model to assess nearby conditions. The target for such collection practice is a total integrated system of top-down instruments from terrestrial sensors to satellite products assimilated with bottom-up inventory models per climate monitoring methodology targets recently proposed to the United Nations Framework Convention on Climate Change for global stocktake. In this presentation, we report preliminary results from on high temporal resolution monitoring of carbon dioxide (CO₂) and methane (CH₄) leaks from an oil & gas extraction site, movement of CO₂ masses with sea air fronts during the NSF TRACER campaign, and CO₂ plume monitoring results from a simulated urban canyon. In this exploratory work, the authors report monitoring real time leaks from gas storage tanks with temporal correlation to site processing time, large gas plumes with temporal drift from rural to urban sites, and scaling factors for simulation scale up of urban canyons from early wind-tunnel studies, respectively. This collection of research narrative illustrates the progress of satellite product assimilation across the rural-urban gradient, with special relevance to greenhouse gas-related industries and policy drivers. For each of these research threads, the prospective research plans will be discussed as well as a total synthesis goal for all projects in the far future.

T23: Synthesis of metal oxide nanoparticles using *Citrus reticulata* for phase and electrochemical study for energy storage application

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Growing interest has been shown in bio-based nanoparticles that are created by employing plant components as ligands to create metal-based compounds. This type of green synthesis incorporates an affordable and environmentally friendly method for producing materials for supercapacitor applications. This work reported a facile synthesis to obtain cobalt oxide nanoparticles (CONPs) using mandarin orange peels. An aqueous extract of orange peels was used as a precursor which inherit a biological reduction mechanism to derive CONPs from cobalt nitrate hexahydrate. Additionally, CONPs were also synthesized by using different precursors for comparative electrochemical activity and charge storing capacity study. Furthermore, the obtained nanoparticles were sulfurized and phosphorized to investigate the effect of morphology and crystalline structure on electrochemical performance. Therefore, various characterization strategy is accompanied. Interestingly, the hybrid capacitor traits were analyzed in 3M basic electrolyte and the bio-derived nanoparticles showed better performance among all. The phosphide sample delivered 106% an improved specific capacitance than sulfide and as such CONPs. Moreover, phosphide-based nanoparticles showed more than 85% capacitance stability after 5000 cycles. In addition, it offers more than 6000 Wh/kg power density with a low charge transfer resistance of 0.70 Ω among all the samples. This study offers a facile strategy to prepare nanosized materials by using plant products for energy application.

T24: Reactive Uptake of Ozone in the Indoor Environment: Commercial Dyes and Respiratory Aerosol

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Ozone is a ubiquitous oxidant in the indoor environment, where Americans spend more than 90% of their time. To understand the role of reactive uptake of ozone to unsaturated species in indoor air chemistry, it is necessary to measure uptake to the wide variety of surfaces present indoors. Many of these surfaces include hygroscopic organic species, whether in films or aerosol particles, for which water may act as a plasticizer, so it is also necessary to measure uptake at a range of ambient relative humidities. Azo dyes are widely used in commercial products, from clothing to cosmetics, and measuring the uptake of ozone onto these species is a crucial first step towards determining potential toxic products of oxidation. Mucin is a representative component of respiratory aerosol, and measuring the uptake of ozone onto this species is vital to understanding the persistence of bacteria and viruses in the indoor environment. Here, we investigate the reactive uptake of ozone on to thin films of azo dyes and mucin in a coated-wall flow-tube. Thin films are prepared on the inner walls of glass tubes and housed in a flow tube with a retractable injector to adjust the amount of surface area exposed to ozone. The uptake onto three azo dyes has been determined to be appreciable, even at 0% relative humidity. The uptake coefficient was higher at 80% relative humidity, consistent with plasticization. The uptake also exhibited an inverse dependence on the ozone mixing ratio, consistent with depletion of unreacted dye near the surface. The uptake was similar for the three dyes, suggesting that it is bulk viscosity that dictates reactive uptake. Uptake coefficients for mucin are about an order of magnitude greater than those for the dyes, under some conditions. These results provide further insights into the complex role of ozone in indoor air chemistry.

T25: Hydrothermal-assisted bi-metallic MOF for hydrogen evolution and energy storage applications

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The most important source to run electrical and electronic devices is energy produced using different structures like composites, MXenes, and Metal-organic frameworks (MOF). Among these structures, MOF has a uniform crystal structure but adjustable porosity, a large surface area, and a good adsorption affinity. These properties made MOFs suitable materials for energy storage applications. As the requirement for rapid energy increases continuously, it results in the development of supercapacitors (SC) and hydrogen generation. These devices possess high power density and high charge storage capacity. This work introduces the highly efficient electrode material derived from nickel (Ni) and cobalt (Co) compounds and their combination for application in SCs and hydrogen evolution reactions (HER). The samples were synthesized using the hydrothermal method at 160 °C, where glutaric acid is used as an organic ligand. The Co-MOF shows the lowest specific capacitance, which is improved by 400% for Ni-MOF, whereas the bi-metallic NiCo-MOF shows more than 500% improvement in C_{sp} compared to the Co-MOF. Furthermore, the catalytic activity has been examined based on HER activity. The Ni and Co-MOF both show 208 mV overpotential at 10 mA/cm², whereas the NiCo-MOF required 182 mV to attain 10 mA/cm² with a Tafel slope of 89 mV/dec. The result demonstrates a new method to fabricate ultrathin and flexible devices using highly efficient MOFs.

T26: Development of Pincer N-Heterocyclic Carbene Ligands Bearing Substituted Pyridine Linker and Their Copper (I) Complexes

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In the field of catalysis, the use of catalysts of precious metals bound by pincer N-heterocyclic carbene ligands is well known. NHC ligands' application in this area is directly related to their ability to strongly bind to the metal thus making the catalysts more stable and less prone to degradation. Recently, there has been growing interests in utilizing more cost-effective, earth abundant metals such as copper and nickel as catalysts in facilitating organic and organometallic transformations. Our group has previously reported Cu(I) complexes supported by unsubstituted pyridyl- and pyridylmethyl-linked pincer NHC ligands that are capable of catalyzing C–C and C–X (X = O, N) coupling reactions (ref 1, 2). We report herein several copper complexes of pincer bis-NHC ligands with substituted pyridine linkers and aim at investigating the effect of the pyridine “R” groups on the coordination chemistry, electronic, and steric properties of these ligands. A particular polynuclear complex could prove to be a useful scaffold to build larger macromolecules tuned for specific reactions. All the complexes have been characterized by HNMR, and X-ray crystallography, DFT studied are ongoing to determine thermodynamic and kinetic factors involved in binding the Cu(I) metal to the pincer bis-NHC ligands.

T27: Polymer-fixed oxidation catalysts for water purification

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Contaminants of Emerging Concern (CEC) are typically anthropogenic organic compounds such as dyes, pesticides, pharmaceuticals, etc., which are becoming increasingly prevalent in wastewater and tend to escape current water purification efforts. In this work, we describe synthetic strategies leading to polymerizable Cu, Fe, and Mn complexes of cross-bridged tetraazamacrocycles. Complexes of this type are known, water stable, broad spectrum homogeneous oxidation catalysts that can use green oxidants, such as hydrogen peroxide and dioxygen, to modify a variety of organic functional groups. In a viable wastewater purification scheme, such catalysts would need to be made heterogeneous so that they can be recycled and used to treat multiple aliquots of wastewater. We are developing monomeric analogues of the known cross-bridged tetraazamacrocycles which have polymerizable pendant arms, with a goal of copolymerization with known polymer types to produce heterogeneous recyclable oxidation catalysts. We present here allyl, benzyl, and primary amine pendant armed cross-bridged tetraazamacrocycles, their Cu, Fe, and Mn complexes, and our progress in producing polymeric materials incorporating them.

T28: Molecular Sculpting; a Versatile Tool for Rapid Access to Various Fluorinated Arenes via Photocatalytic Hydrodefluorination of Benzoates

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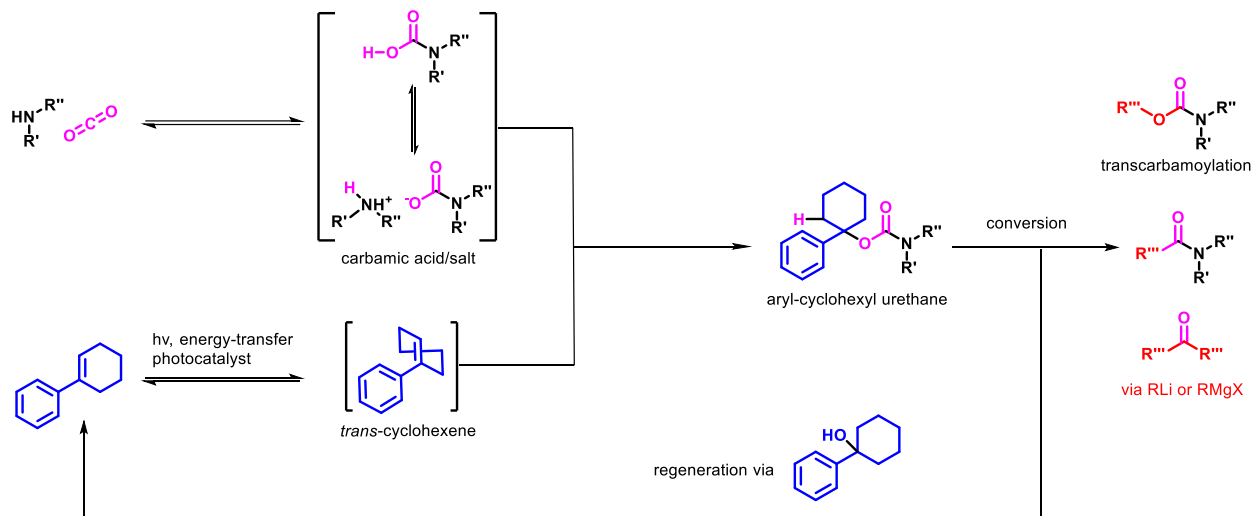
Starting with highly fluorinated benzoates, we develop the directed photocatalytic hydrodefluorination (HDF) of fluorinated aryl benzoates and demonstrate its synergistic use with other HDF strategies, along with C–H arylation, decarboxylative coupling and decarboxylative protonation to access most fluorination patterns found in benzoate derivatives and by extension, benzene derivatives *via* a molecular sculpting approach. Mild reaction conditions and excellent regioselectivity make the approach ideal for synthesis. This approach provides access to 16 benzoate derivatives with different fluorination patterns from just a couple of highly fluorinated, commercially available benzoic acids. We synthesize key intermediates or the API for sitagliptin, diflunisal, and other pharmaceutically important molecules. Importantly, we provide key insights into relative rates of defluorination and strategies to alter these rates. We provide demonstrations of the synergistic use of HDF and related technologies to rapidly enhance the synthetic complexity of these simple commercially available perfluoroarenes into complex partially fluorinated molecules.

T29: Urethanes from CO₂ and Visible Light: Putting Molecular Strain to Work

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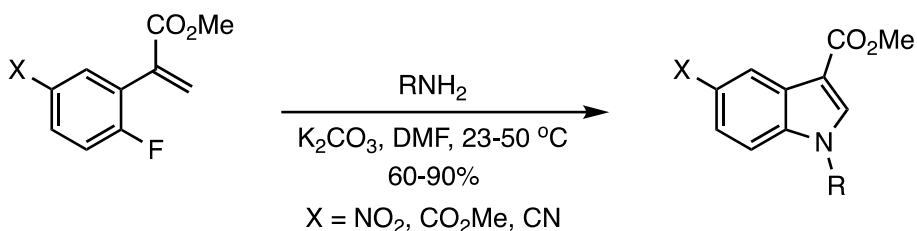


Furthering the idea of using molecular strain as a synthetic energy currency, a visible-light photocatalytic method has been investigated for the capture of CO₂ as urethanes. Ordinarily, late-stage, modular installation of alkyl and aryl urethanes is realized through high-oxidation-state C1 synthons such as chloroformates, alkyl carbonates, and CO. Methods utilizing CO₂ necessarily require high-energy electrophilic molecules to form carbamates - trans-cyclohexenes in the case of this research. A scope of primary and secondary amines was treated with CO₂ and the resultant ammonium carbamate salts were intercepted by a series of photoexcited aryl cyclohexenes. The resulting urethanes were then demonstrated as flexible intermediates other urethanes, carboxamides, and ketones.

T30: Domino Aza-Michael Addition-S_NAr-Heteroaromatization Route to C5-Substituted 1-Alkyl-1*H*-indole-3-carboxylic Esters

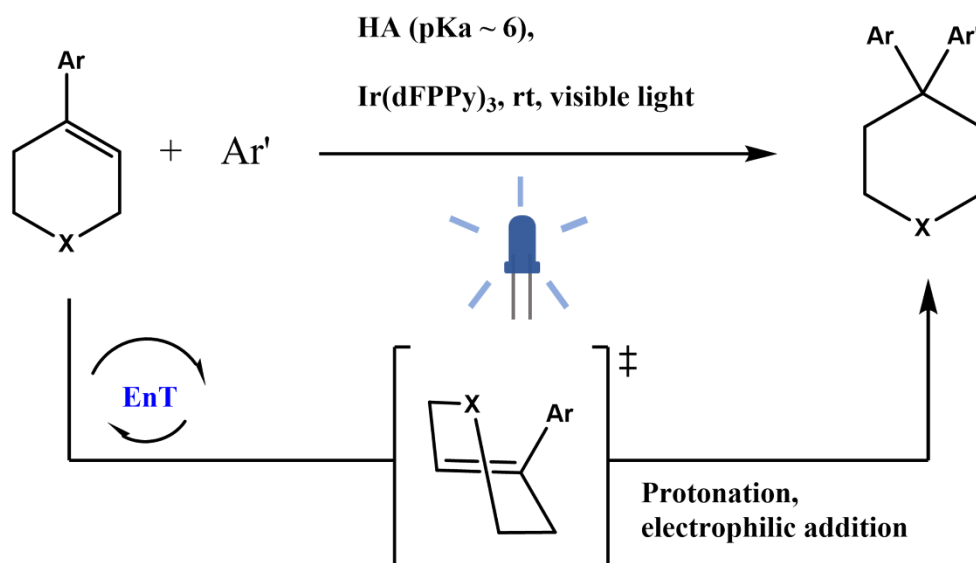
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A new synthesis of C5-substituted 1-alkyl-1*H*-indole-3-carboxylic esters is reported. A series of styrene derivatives, substituted to activate them toward aza-Michael addition and S_NAr reaction were prepared. Subsequent reaction with a series of primary amines generated the title compounds. The reaction proceeded in DMF at 23-50 °C using equimolar quantities of the activated styrene and the amine with 2 equivalents of K₂CO₃ to give 60-90% of the indole products. The reaction involves an aza-Michael addition, followed by S_NAr ring closure and heteroaromatization. Since the reactions were run under nitrogen, the final oxidation likely results from dissolved oxygen in the DMF. Substrates incorporating a nitrile in the styryl side chain proved too reactive to use in this sequence. The synthesis of the reaction substrates, their relative reactivities, and mechanistic details of the reaction will be discussed.



T31: Twisting the limits of Friedel-Crafts chemistry: Access to quaternary, diaryl, cycles through visible light photocatalysis

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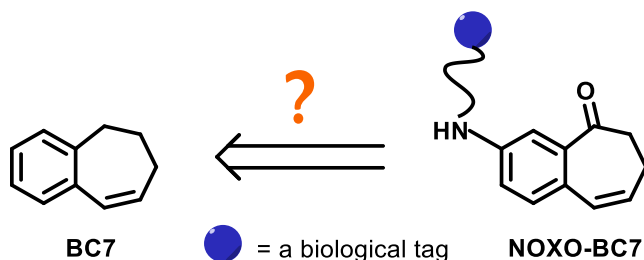


There has been considerable effort over the last century and a half to form C-C bonds through the development of palladium catalyzed cross-coupling reagents, organocatalysts, Friedel-Crafts chemistry, boronic acids and esters, recently thianthrenes and much, much, more. In recent years, organic chemistry has been pushed toward more practical conditions, utilizing powerful catalysts and mild reaction conditions. Friedel-Crafts chemistry has witnessed only minor adaptation from the traditional conditions. This work captures the essence of Friedel-Crafts chemistry but with a “twist”. This chemistry appropriates a transient, highly strained, trans-cyclohexene derived tertiary carbenium, promoted through a dexter-energy transfer from an efficient photo-catalyst. Our chemistry has achieved an array of useful diaryl-quaternary carbon centers from both hetero and carbocyclic nucleophiles and starting materials, including some notable neuropharmacological motifs.

T32: Synthesis of NOXO-BC7

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The click reactions which have fast kinetics and that are bio-orthogonal have been used in bioconjugation to help study complex biological systems. When light can be used to trigger the chemistry this provides both spatial and temporal control. In the recent past, the Weaver research group demonstrated that when benzocycloheptene (**BC7**) was in the presence of a photocatalyst, it is capable of converting visible light into strain energy. They demonstrated that this strain energy could facilitate cycloaddition of azides to give non-aromatic triazolone products under very mild conditions that were amenable to bioconjugation. To advance this technology, it became clear that a molecule like the aminoxo analog, shown below, was needed. This talk will discuss the various routes that have been explored before finding a successful route to synthesize **NOXO-BC7**.



T33: Theoretical Investigation of Metal Doped Gold Nano-Clusters $M@Au_n$ ($M = W, Co, \text{ and } Ir$)

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Gold nanoclusters have attracted considerable interest over the past two decades due to their wide applications as catalysts, sensors, molecular electronics, and bioconjugate probes for amplification tags in gene analysis, antibody or antigen detection, DNA sequencing, and gene mapping. One of the major interests of cluster science is to discover highly stable clusters, which may be used as building blocks for novel materials.

The structures and stabilities of endohedral gold clusters $M@Au_n$ ($M=W, Co, \text{ and } Ir$) have been studied with density functional theory (DFT). The local density approximation (LDA) functional SVWN, the generalized gradient approximation (GGA) functional BP86, and PBE/PBE and the hybrid density functional B3LYP and PBE1PBE were employed to calculate the embedding energies, binding energies, ionization potentials, and electron affinities for these clusters. The effective core potential and corresponding valence basis set LanL2DZ and LanL2TZ were used throughout the calculations. The $M@Au_n$ ($M = W, Co, Ir$) clusters have higher binding energies than the empty Au_n cluster, indicating that doping with a transition metal atom into the unstable Au_n cage cluster stabilizes the hollow cage structure. In this meeting, the theoretically calculated results of $M@Au_n$ ($M = W, Co, Ir$) clusters will be presented.

T34: Hydrogen Peroxide Vapor Detection Using Low-Cost Thin Film

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One method for colorimetric detection of hydrogen peroxide vapor is based on a titanium hydrogen peroxide complex. Xplosafe's XploSens PS commercial titanium(IV)-based peroxide gas detection test strips are used to detect hydrogen peroxide gas using low-cost hardware. The exposure of these test strips to hydrogen peroxide liquid or gas leads to the development of an intense yellow or orange color. For hydrogen peroxide gas, an inexpensive web camera and a tungsten lamp were used to measure the reflected light intensity as a function of exposure time from a test strip held in a custom cell. The measured rate of color change indicates high sensitivity and first order kinetics over a hydrogen peroxide concentration range of approximately 2 to 30 ppm by volume. For a 1-min measurement, the gas-phase detection limit is estimated to be 1 ppm. A 0.01 ppm detection limit can be obtained with a 1-h exposure time. Titanium(IV)-based peroxide detection test strips are sensitive enough to work as a gas-phase hydrogen peroxide detector. Current research is looking at the addition of an acid reagent, trifluoromethanesulfonic acid, adsorbed onto low-cost silicone TLC plates to enhance the sensor activity towards the peroxide gas detection. These new materials are a starting point for the preparation of more active sensor materials for the hydrogen peroxide and organic peroxide vapor detection.

T35: Transferability of Machine Learning Potentials for Solution-Phase Reactions

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In recent years, rapid progresses have been made in developing machine learning potentials (MLPs) to reproduce high-quality potential energy surfaces for chemical systems. However, the transferability is still a limiting factor for their broad applications, especially for the system-specific MLPs. Recently, we developed QM/MM-like MLPs [J. Chem. Theory Comput. 2021, 17, 9, 5745–5758] to reproduce *ab initio* quantum-mechanical/molecular-mechanical (ai-QM/MM) potential energy surfaces for the Menshutkin reaction in water and the chorismate mutase reaction, which were then used to calculate the free energy profiles for the corresponding reactions. The objective of the current study is to investigate the transferability of the MLPs in different solvents. To achieve this, we trained a MLP for an S_N2 reaction (CH₃Br + Cl⁻ → CH₃Cl + Br⁻) in water, and tested its accuracies in other solvents (dimethylformamide, methanol, and acetone) without further trainings. The results showed that good transferability could be achieved when changing the solvent environment, which paves the way for exploring the possibility that for enzymatic reactions, a MLP trained for the wild-type system could be transferred to study the reaction in its mutants.

T36: Post-consumer polypropylene carpet and mixed polyolefin waste make structural composites

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Around 90% of carpet waste is discarded in landfills, 6% is incinerated, and less than 5% is recycled in the U.S. Most plastic bottles are made from polyethylene terephthalate (PET) resin which can easily be recycled, unlike bottle caps, usually polyolefins, which are often mixed with other materials (like labels, ink, and remnant products). These are problematic to recycle. Processing the discarded materials to form new and valuable composites can add additional value to materials that would otherwise end up in a landfill. As a part of a larger research project, we are making composites using post-consumer polypropylene carpets (c-PP) and mixed polyolefins recovered from post-consumer bottle waste by compression molding. A comparison of composites made from different polyolefins and polyolefins with different purity levels will be reported. The effect of carpet level of wear on the mechanical properties of the composites was also examined. The quality of the molded samples was characterized by flexural strength and modulus, creep behavior, impact strength, fastener holding capability, and microscopic images. We find that these samples can have useful mechanical properties and possibly be useful for structural applications.

T37: Plant-based Polyol and further Polyurethane/ Graphene-based Composites to Study the Increasing Mechanical Strength

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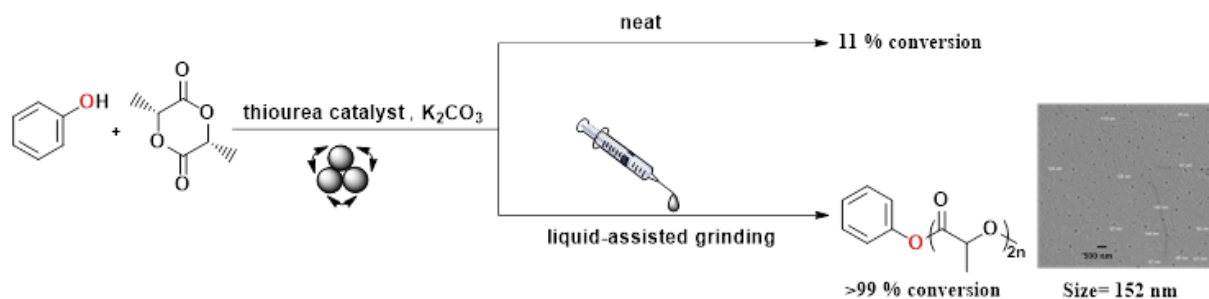
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Using different starting materials to produce polyurethanes (PU) - is the only approach that makes PU unique among all other polymers. This approach enriches the PU with a wide selection of properties to develop a variety of forms such as coatings, adhesives, and foams. In that, petroleum-based polyol, which is the main component of PU, is delivering a harmful impact on the environment. Also, petroleum sources are non-renewable and expensive. As a solution to that, researchers are taking advantage of renewable resources such as soybean, and limonene to use as raw materials in the preparation of polyols. As a green synthesis route, sunflower oil was used in this work to make polyol by using epoxidation and ring-opening reaction mechanisms. The synthesized polyol was further confirmed by standard techniques of FT-IR, GPC, and OH value. After the confirmation of synthesis, polyurethane films were prepared with the addition of isocyanate and four different graphene-based composites. Graphene oxide (GO), reduced graphene oxide (rGO), graphene nanoplatelets (GNPs), and graphene nanoribbons (GNR) were dispersed into the polyol as composites. The samples were prepared by dispersing 0.01, 0.02, and 0.05 wt.% of graphene. After curing at a certain temperature, various mechanical and thermal tests were performed to examine the properties of PU films. As a result, the thermal stability was increased slightly. In terms of mechanical strength, the tensile stress applied to the sample was increased from neat PU (9 MPa) to PU/GNP (35 MPa). The hardness was also increased from shore D hardness 51 to 70. This work examined the effect of different additives with plant-based PUs, in terms of mechanical strength.

T38: One Pot Phenolic-Initiated Mechanochemical Synthesis of Poly(lactic acid) Nanoparticles

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Due to its biodegradable and biocompatible nature, polylactic acid (PLA) has found widespread use in biomedical applications. Controlled drug delivery using PLA-based nanoparticles (PLA-NPs) is an important tool for tuning the bioavailability of therapeutics. Traditional methods to prepare PLA-NPs require a multistep process that is time-consuming and produces significant aqueous and organic waste streams. This work reports a one-pot mechanochemical synthesis of lactide to PLA-NPs. Our results demonstrate a robust and optimized one-pot method for preparing precisely defined nanoparticles which generates minimal waste.



T39: Biodegradable Aliphatic Polyesters Synthesized *via* Melt-Polycondensation

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Ever-growing concerns have been raised about the detrimental impacts caused by the continually increasing volume of environment-persistent plastic wastes, globally. Consequently, synthetic biodegradable polymers have gained substantial research and industrial devotion, potentially substituting non-biodegradable synthetic polymers in widespread applications. Biodegradable aliphatic polyesters synthesized *via* ring opening polymerization of cyclic- lactones, lactides, and carbonates, and *via* polycondensation of diacids and diols have been highly valued. This research, therefore, aims to synthesize the biodegradable aliphatic polyesters *via* melt-polycondensation using the monomers primarily derived from waste plastics or bio-based resources instead of petrochemical derivatives. As proof of concept, commercially available precursors were used for synthesizing the aliphatic polyesters *via* melt-polycondensation. Specifically, the aliphatic polyesters were synthesized using dimethyl sebacate (DMS) and diols (ethylene glycol, 1,3-propane diol, or 1,5-pentadiol). The effect of stoichiometric ratio (DMS to diol), polymerization conditions (time, temperature, and pressure; ambient or reduced), and catalyst (stannous octoate and/or titanium isopropoxide) were investigated. The synthesized polyesters were purified by dissolution and re-precipitation method (chloroform and methanol, respectively), and characterized using gel permeation chromatography, Fourier transform-infrared spectroscopy (FT-IR), differential scanning calorimeter (DSC), and thermal gravimetric analyzer (TGA). Characteristic peaks of aliphatic polyesters were observed in the FT-IR spectra, and both the catalysts produced polyesters with comparable molecular weights and low dispersity. Increasing the melt-polycondensation temperatures over 240 °C caused the yellowing of polyesters. The DSC and TGA thermograms showed temperatures of melting, crystallization, and onset thermal degradation similar to that reported in the literature. The findings suggest that the catalyst, stannous octoate generally applied for ring-opening polymerization may be satisfactorily employed for synthesizing the biodegradable aliphatic polyesters *via* melt-polycondensation.

T40: Effect of crystallinity on mechanical properties of poly(ethylene terephthalate) (PET)

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Poly(ethylene terephthalate) (PET) is a widely used polymer in the food packaging industry due to its unique mechanical and thermal properties together with relatively low production cost. PET is a common thermoplastic polymer of polyester family often made by the polycondensation of terephthalic acid and ethylene glycol. The semicrystalline nature of PET primarily contributes to its desirable physical and chemical properties. PET sheets were made by compression molding. Annealing and quenching at different temperatures during the molding process, allowed samples with different crystallinity to be made. The crystallinity amounts were calculated from the differential scanning calorimetry (DSC) data. A trend in the crystallinity of PET with respect to the quenching temperatures was observed. Three-point flexural bending test was performed to determine the effect of different amounts of crystallinity on the flexural strength and modulus of the molded samples. The three-point flexural data indicated that the flexural strength and modulus of the samples change with respect to the PET crystallinity.

T41: Facile Mechanochemical Suzuki Polymerization for the Synthesis of Polyfluorenes

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Polyfluorenes are considered as one of the most attractive blue-light emitting materials due to their charge transport properties, high efficiency, high chemical and thermal stability, high solubility, film-forming ability, and good tunability through chemical modification and copolymerization.¹ Nevertheless, most of the synthetic routes for these compounds are costly and requires large amounts of solvent, energy, and catalysts. Herein, the synthesis of poly(9,9-di-n-octylfluorenyl-2,7-diyl) (PF), poly(9,9-dioctylfluorene-alt-benzothiadiazole) (PFBT), poly[(9,9-bis(3'-(N,N-dimethylamino)propyl)-2,7-fluorene)alt-2,7-(9,9-dioctylfluorene)] (PFN) are reported by an catalytic Suzuki-Miyaura polymerization in the ball-mill will be presented.² This synthesis technique yields polyfluorene and its derivatives in 30 minutes or less milling time. Furthermore, the polymer light emitting diode and photovoltaic interfacial electrolyte, poly(9,9-bis(3'-(N,N-dimethyl)-N-ethylammonium-propyl-2,7-fluorene)-alt-2,7-(9,9-dioctylfluorene))dibromide (PFN-Br) was obtained by using a simple and rapid mechanochemical quaternization reaction of PFN will also be presented.

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T42: Novel openings in utilization of animal waste for polyurethane industries

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Growing environmental awareness, the recycling of waste materials into valuable forms has become one of the hot topics in this era. The use of low-cost, bio-renewable materials for the development of value-added products is highly desired by many industries, particularly polyurethanes. The amount of chicken waste produced in the United States is staggering, and chicken fat is a valuable by-product of chicken waste and is currently used for a variety of useful purposes. In this work, we synthesized a chicken fat-based polyol through epoxidation followed by a ring-opening approach to make polyurethane foams (PUF). The high unsaturated fatty acids content in the chicken fat makes it a prospective alternative source for greener polyurethane formation. The high flammability of PUF is one of the major concerns whether they are synthesized using petrochemical or biobased materials. To reduce the flammability of PUF, dimethyl methylphosphonate (DMMP), a P-based flame retardant (FR) was introduced. The mechanical and thermal characteristics of PUFs were studied using density, closed-cell content, cell distribution, thermal stability, and horizontal burning parameters. PUFs maintained their structure regardless of the addition of DMMP, suggesting that there is a proper interaction between the active FR compound along with the biobased PUF matrix. Moreover, chicken fat-based polyol served as a viable material for making FR- rigid PUF as it delivered satisfactory properties for its mechanical and thermal behavior. The incorporation of this type of waste material into PUF synthesis showed novel possibilities for using animal waste as a sustainable option for polyurethane industries.

T43: Parameters effecting mechanical properties of composites from post-consumer polyester carpet and recycled PET resin.

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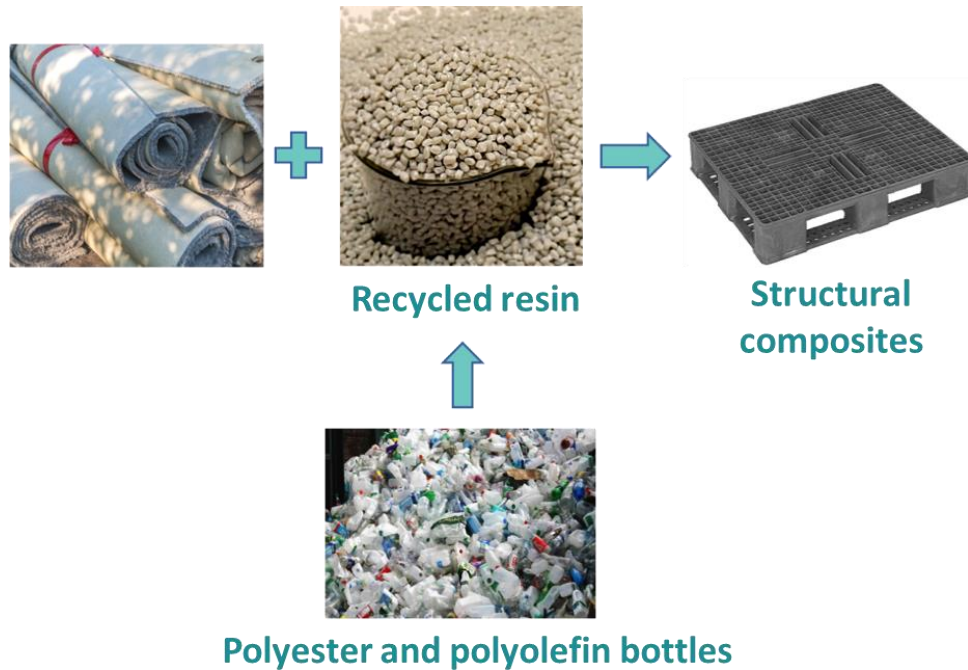
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A method was developed for fabricating recycled composites from post-consumer polyethylene terephthalate (PET) carpets and recycled PET resins. Compression molding of the components under different pressures, temperatures, and component layups was performed. Preliminary molding conditions were arrived at based on analyzing the differential scanning calorimetry (DSC), thermal gravimetric analysis (TGA), and melt viscosity data for different raw material combinations. Molding factors were screened to define applicable ranges for each parameter. The effects of configuration and composition of components, temperature, molding time, and pressure were considered in the screening process. Mechanical properties of composites were determined by 3-point flexural (according to ASTM D790) and creep tests. The molded materials showed acceptable mechanical strength and modulus values required for structural applications.



Poster Abstracts

P1: Spectrophotometric Determination of Metal Complex pK_a s

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The use of natural and unnatural amino acids has many biomedically related applications, some of which include, tissue engineering, drug design and delivery and mutagenesis. The obstacle to overcome is the development of synthetic means to generate natural and unnatural amino acids. The synthetic method our collaborators use relies on metal complexation of a glycine Schiff's Base to protect the amino and carboxyl groups of the glycine. They have shown an improvement to this method which involves metal complexed Schiff's bases of glycine which contain an electron withdrawing groups. The addition of electron withdrawing groups is hypothesized to increase the acidity of the C-H Bond on the α -carbon of the glycine, thus allowing for milder conditions to be used while increasing the generality and efficiency in creating the desired amino acids. To test this hypothesis, a series of glycine metal complexes have been synthesized. Spectroscopic methods were used to quantify the pK_a changes corresponding to the addition of electron withdrawing groups to the metal complexed Schiff's base of glycine. Obstacles faced in determining the pK_a 's of each ligand include monitoring of a weak acid-weak base chemical reaction, reaction solvent system, the barrier of Le Châtelier's principle in certain solvent systems, and the use of different methods to determine the acidity of a proton in organic solvent conditions, since aqueous methods are not possible. We have been able to determine the ΔpK_a of the C-H proton on the glycine in the metal complexes when compared to a methanol/methoxide acid/base system. The pK_a of the methanol has been established as 15.5. Currently we are evaluating different solvent systems for further studies.

P2: Optimization of Higher-Energy Collisional Dissociation Fragmentation Energy for Intact Protein-level Tandem Mass Tag Labeling

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Isobaric chemical tag labeling [e.g., iTRAQ and Tandem Mass Tag (TMT)] is a commonly used approach in quantitative proteomics research. Typically, peptides are labeled with covalent chemical tags and quantified through detection of low-mass reporter ions generated after MS2 fragmentation during tandem mass spectrometry (MS/MS). Recently, we introduced and optimized a platform for intact protein-level TMT labeling for identification and quantification that demonstrated >90% labeling efficiency in complex samples with top-down proteomics. MS2 fragmentation is used to simultaneously fragment peptides and proteins for identification and cleave reporter ions for quantitation. Then, higher-energy collisional dissociation (HCD), a popular fragmentation method that produces accurate reporter ion intensities and avoids the loss of low mass ions, is used. HCD energies have been optimized for peptide-level isobaric chemical tag labeling; however, fragmentation energies have not been evaluated for TMT-labeled intact proteins to balance protein identification and energies on TMT-labeled *HeLa* lysate with top-down proteomics.

In our study, we used *HeLa* cell lysate to analyze the effects of different HCD energies in reporter ion fragmentation and protein identification. *HeLa* cell lysate was reduced (TCEP), alkylated (IAA), buffer exchanged to TEAB buffer, and then TMT labeled using optimized conditions as previously reported (Guo et al. 2022). The TMT-labeled sample was separated by C2 capillary column and subjected to MS/MS using an Orbitrap Exploris 240 mass spectrometer with varying HCD energies (25%, 30%, 35%, 40%, 45%, 50%, 80%; stepped HCD energies 30%, 40%, 50%, and 35%, 45%, 50%). An in-house python package and TopPIC Suite was used for reporter ion intensity extraction and proteoform identification, respectively.

Parameters including reporter ion intensities, E-value, matched peaks, PrSM, and proteoform counts were compared across different HCD energies to evaluate quantification and identification. Our results indicated that (1) as HCD fragmentation energy increased (HCD 25%-80%), reporter ion intensity also increased and stepped HCD generated similar reporter ion intensities to HCD 45%. (2) Identification confidence increased as HCD energy increased from 35% to 45%, though it decreased at 50 and 80%. The two stepped HCD analyses outperformed the single energy analyses and also showed low run-to-run variability. (3) The number of matched peaks and fragment ions also increased from 25-45% and decreased at 50 and 80%. (4) The PrSM count increased from 25-40% and remained approximately constant for 40, 45, and 50% with approximately 800 PrSM counts; however stepped HCD outperformed the discreet energy analyses, resulting in more than 1000 PrSM counts.

Overall, our study demonstrated that stepped HCD fragmentation energy between 30 and 50% resulted in optimized quantitation and identification for TMT-labeled intact protein lysate.

P3: The Effect of HK2 on Lymphatic Vessel Development

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The proper proliferation of lymphatic vessels, or lymphangiogenesis, is critical for the different functions of the lymphatic system: immune response, maintenance of blood flow, and transportation of fatty acids among other roles. A variety of signaling molecules regulate lymphangiogenesis, with the primary ones being SOX18, Coup-TFII, and transcription factor PROX1. PROX1 indirectly affects the levels of vascular endothelial growth factor receptor 3 (VEGFR3), a receptor for one of the VEGF growth factors, through the induction of a set of genes, such as FLT4, that play a role in lymphatic endothelial cell growth and differentiation. Additionally, data suggests VEGFC signaling cross-talks with FGF2 (fibroblast growth factor), making both important for lymphatic development. One important factor that regulates lymphatic vessel growth are the various types of typical metabolism present. Fatty acid oxidation (FAO) is the breakdown of fatty acids into acetyl-CoA, which is ultimately used in the different steps of cellular respiration. This process allows PROX1 to access and activate FLT4. Similarly, hexokinase 2 (HK2) is an enzyme important for the phosphorylation of glucose to glucose-6-phosphate, the first step in glycolysis. Currently, FGF signaling stimulates the transcription of HK2 which is important for producing energy in endothelial cells and promoting growth. Through the manipulation of metabolic pathways and enzymes, novel therapeutics and gene targeting techniques can be used to help with diseases such as edema, cancer, inflammation, and heart failure.

P4: Synthesis of Gold Nanoparticles

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Synthesis of nanoparticles such as gold nanorods (GNRs) have unique characteristics that allow the potential of use in various fields of nanotechnology. The process to synthesize GNRs occurs in a three-step process. The first to this is the formation of the seed solution where chlorauric acid (HAuCl_4), hexadecyltrimethylammonium bromide (CTAB), and sodium borohydride (NaBH_4) to form electron dense micelles. The second step creates a growth solution by combining reducing agents and aromatic salts to create an environment so micelles can form rods. For this the seed and growth solution are combined and the gold is reduced. By using Uv-vis the absorbance can be analyzed to determine the formation of the rods as well as the Transverse (diameter) and Longitudinal (length) aspects to determine the size of the nanoparticles.

P5: Quality Control Systems with HLA DP

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Human leukocyte antigens (HLA) are genes in the major histocompatibility complex (MHC) that help code for proteins that differentiate between “self” and “non-self.” They play a significant role in disease and immune defense. Pure Protein is one of a few companies that are pioneering research with soluble HLA specifically for the HLA DP subtype, one of the biomarkers in transplantation. Clinically, transplant patients can develop detrimental antibodies against their received organ, leading to rejection. Therefore, it is of utmost importance that doctors can recognize these HLA rejection-causing antibodies before they destroy the new organ. Doctors usually test for rejection with tissue-type tests using HLA Markers like HLA DP. Within my research, a major goal is to validate a set of distinct target DP proteins by developing a quality control system to test their effectiveness in recognizing DP antibodies and performing testing to obtain quantitative data that can be used to develop a risk assessment model. The development of a DP antibody detection system is based on ELISA technology. To mimic a human cell carrying specific HLA molecules, we use a plastic chamber that contains immobilized soluble HLA attached through a specific bonding mechanism. Thereafter, either specific quality control antibodies are added to confirm the DP molecule target or serological antibodies from patients to determine their rejection potency.

P6: Cloning of Human cDNA into the Lentiviral Vector

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The ability to manipulate bacterial plasmids greatly advanced the field of molecular biology. The aim of this project is to explore how to use plasmid vector and bacteria to subclone human cDNA into Lentiviral vector. We aimed to clone wildtype and mutant ATAD3A cDNA into the Lentiviral vector. We performed PCR to amplify ATAD3A cDNA using primers carrying restriction enzyme sites. Then, we digested the PCR DNA with the restriction enzymes. This DNA was ligated into the Lentiviral vector using a DNA ligase. This results in a plasmid that E.coli cells can uptake during electroporation. As the E.coli cells multiplied during inoculation, the bacterial cells made copies of the plasmid into each new cell. The plasmids was isolated from the bacterial cells. This process amplified the number of the lentiviral vector containing the human ATAD3A cDNA. The resulting plasmids will be used for transfection, where they are introduced to target cells that express the human cDNA. The process of subcloning is versatile, with much room for manipulation. cDNA can be chosen from any protein coding sequence to analyze protein structures and functions.

P7: Hydroxamic Acid Compounds for Inhibition of Metallo- β -Lactamase from *Bacillus anthracis*

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The emergence of resistant bacteria takes place, endangering the effectiveness of antibiotics. A reason for antibiotic resistance is the presence of lactamases that catalyze the hydrolysis of β -lactam antibiotics. An inhibitor of serine- β -lactamases such as clavulanic acid binds to the active site of the enzymes, thus solving the resistance problem. A pressing issue, however, is that the reaction mechanism of metallo- β -lactamases (MBLs) hydrolyzing β -lactam antibiotics differs from that of serine- β -lactamases due to the existence of zinc ions in the active site of MBLs. Thus, the development of potential inhibitors for MBLs remains urgent. Here, the ability to inhibit MBL from *Bacillus anthracis* (Bla₂) was investigated in silico and in vitro using compounds possessing two hydroxamate functional groups such as 3-chloro-N-hydroxy-4-(7-(hydroxyamino)-7-oxoheptyl) benzamide (Compound **4**) and N-hydroxy-4-(7-(hydroxyamino)-7-oxoheptyl)-3-methoxybenzamide (Compound **6**). In silico docking and molecular dynamics simulations revealed that both Compounds **4** and **6** were coordinated with zinc ions in the active site, suggesting that the hydroxamate group attached to the aromatic ring of the compound plays a crucial role in the coordination to the zinc ions. In vitro kinetic analysis demonstrated that the mode of inhibitions for Compounds **4** and **6** were a competitive inhibition with K_i values of 6.4 ± 1.7 and 4.7 ± 1.4 μ M, respectively. The agreement between in silico and in vitro investigations indicates that compounds containing dihydroxamate moieties may offer a new avenue to overcome antibiotic resistance to bacteria.

P8: Expression, Purification, and Glycosylation of γ -sarcoglycan

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Due to its role in maintaining the structural integrity of muscle cell sarcolemma, γ -sarcoglycan, when deficient, or mutated in cells, results in Limb-Girdle Muscular Dystrophy. γ -sarcoglycan is extremely difficult to express and purify even in milligram quantities due to its hydrophobic nature making it difficult to study and for this reason, not much work on the structure, and dynamics of this protein. We show here the expression of full length recombinant γ -sarcoglycan in *Escherichia coli*, its purification using size exclusion chromatography, and the incorporation of the protein in detergents and lipids that mimic the natural membrane environment of the protein.

It has been suggested that the adding a sugar molecule to a protein, through glycosylation, has a direct effect on how the protein folds, its interactions with other biomolecules, and the overall function of the protein. Glycoproteins play key roles in a myriad of biological processes and are estimated to form as high as 50% of human proteins. This makes glycosylation (the attachment of sugar) an essential post-translational modification in proteins. Here, we show the successful *in vitro* glycosylation of full length γ -sarcoglycan with N-glycosyltransferase (NGT), again using detergents that mimic the native environment of γ -sarcoglycan in order to test whether glycosylation does in fact change protein structure, dynamics and protein-protein interactions.

P9: Inhibition of Metallo-beta-lactamase from *Bacillus anthracis* by Hydroxybenzoic Acid

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Anthrax, caused by *Bacillus anthracis*, can be treated with antibiotics such as tetracyclines, macrolides, quinolones, and β -lactams. However, studies have shown that *B. anthracis* isolates can show variable sensitivity to multiple classes of antibiotics. *B. anthracis* carry chromosomal genes *bla1* and *bla2*, which give β -lactam resistance. The gene *bla2* encodes for metallo- β -lactamase containing zinc ions providing resistance to most β -lactam antibiotics such as penicillins and cephalosporins. Furthermore, there are no commercially available inhibitors for metallo- β -lactamase unlike clavulanic acid for non-metallo- β -lactamases encoded by the gene *bla1*. Here, we attempted to explore the possibility of any inhibition by aspirin given that aspirin is relatively less toxic and contains carboxyl group that could bind to zinc ions. However, according to computational analyses, aspirin appears to be unable to bind to the zinc ions in the active site pocket whereas an aspirin analog (4-acetyloxybenzoic acid) was able to bind to the zinc ions. We successfully synthesized the aspirin analog, confirmed by TLC, IR and NMR. This analog may give us an idea how to develop effective inhibitors for metallo- β -lactamases.

P10: Synthesizing Aspirin Analogs to Inhibit HDAC1

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The deacetylation by histone deacetylases (HDACs) is important in epigenetic, non-epigenetic, and regulation. Hyperacetylation takes place as HDACs are inhibited, thus leading to the transcriptional activation of a number of genes. HDACs have emerged as targets for anticancer drug development because HDAC inhibitors has been known to prevent the formation of malignant tumors. This research focused on synthesizing aspirin analogs to inhibit HDAC1, an HDAC containing a zinc ion as cofactor, given that the aspirin analogs contain a zinc ion binding functional group – i.e., carboxylate. We showed the binding between HDAC1 and an aspirin analog using computational analysis and confirmed the synthesis by TLC, IR and NMR.

P11: Mechanisms of Resveratrol in Inhibiting Cancer

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Resveratrol is a naturally occurring phenol that is synthesized in plants and found in food sources such as grapes, blueberries, and peanuts. Resveratrol contains two phenol rings connected by an ethylene bridge and has close to 100 naturally occurring oligomers. The hydroxyl groups present in resveratrol enable its interaction with proteins and other nutrients. Though resveratrol demonstrates lipophilic traits which aid in its absorption into the cell, its hydrophobicity and restricted solubility in water decrease its oral bioavailability, thereby limiting the drug's effectiveness. Experiments have confirmed resveratrol's role in inhibiting all stages of carcinogenesis, including initiation, promotion, and progression. Resveratrol is also known to be anti-inflammatory, cardioprotective, neuroprotective, vasorelaxant, phytoestrogenic, etc., making it an important biological compound. In addition to various cancers, resveratrol is also useful in treating other diseases including cardiovascular diseases, neurological diseases such as strokes, ischemia, and Huntington's disease, and Alzheimer's.

The unique structure of resveratrol allows it to target not only multiple types of cancer, but also limit tumorigenesis through both a p53 dependent and independent pathways. Through one particular p53 independent pathway, a western blot analysis showed that resveratrol enables the activation of transcription factors NF- κ B and AP-1, resulting in the downregulation of cancer-driving genes and the limitation of oncogenesis. In addition to being able to engage in both p53 independent and dependent mechanisms, the compound's unique chemical and physical properties allow it to interact with cancer cells through both intracellular mechanisms and signaling pathways. Resveratrol takes an intracellular route by inducing kinase inhibitor proteins p21^{WAS/CIP1}, p21^{KIP1}, and p57^{KIP2}, which then bind to D/E cyclin dependent kinases that block the cell's S/G1 phase and ultimately inhibit cell cycle progression. Using a signaling pathway, resveratrol binds to the cell membrane receptor integrin $\alpha\beta3$. Through a western blot for p53 detection, it was found that integrin $\alpha\beta3$ activated mitogen-activated protein kinase and the serine phosphorylation p53 in cancer cells, resulting in the activation of extracellular signal-regulated kinases 1 and 2, and therefore oncogenesis limitation.

Resveratrol's ability to limit tumorigenesis through multiple pathways shows great potential for further cancer prevention efforts. The compound's poor bioavailability reduces its anticancer effects, so further research must be done on improving its bioavailability and optimizing an oncogenesis suppression method. Researchers must also look further in order to understand the effects of resveratrol's derivatives on cancer cells, as resveratrol's metabolites may have greater bioavailability, plasma levels, and tissue concentrations.

P12: An Eco-Friendly method to disrupt Pheromones in *Ostrina Nubilalis*: Helping hand to farmers.

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European corn borer (ECB) *Ostrinia nubilalis* (Onub), is a very serious pest of corn, sweet corn, and other crops. ECB accounts for 5.5 to 8.5 million tons of corn loss in an average year in Europe and other countries. ECB was introduced to the United States in the 1900s. This pest accounts for 20% of yield loss in North America with damages estimated to exceed the US \$1 billion annually. Pesticides and insecticides used to control these pests cause harmful effects on the environment. Moreover, pests show resistance to it. Thus, there is an urgent need for an alternate method of pest control. Mating in lepidopteran moths such as *Ostrinia nubilalis* is initiated with the detection of female-secreted pheromones by the males. The pheromone binding proteins (PBPs) present in the male moth antenna play a critical role in pheromone detection. Of the five PBPs identified in *Ostrinia nubilalis*, OnubPBP2 and OnubPBP3 have male-biased expression. An alternate approach for pest control is to target the mating process by intervening in the pheromone detection system of the male moth. Structure-function study of the OnubPBP2 is critical to interfere in the pheromone detection system of this invasive insect pest in a species-specific and environmentally friendly manner. To achieve this goal, we have cloned, expressed, purified, and investigated the recombinant OnubPBP2 through biophysical characterization. We have determined the high-resolution 3-dimensional structure of OnubPBP2 by NMR spectroscopy.

P13: CONJUGATING MODIFIED DNA TO THIOLATED SILICA NANOPARTICLES TOWARDS NANOPARTICLE SELF-ASSEMBLY

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Introduction: Silica nanoparticles (SiNPs) exhibit high stability, low toxicity, and a large surface area to volume ratio, making them viable biocompatible carriers and biomarkers with significant potential for surface functionalization. Modifying functionalized SiNPs with custom ssDNA oligos allows for a system of self-assembly that effectuates controlled nanostructure formation via base pairing. This “bottom-up” approach enables greater spatial control in tuning the size and shape of nanostructures — a feature important for cellular-targeting in drug delivery systems — compared with “top-down” approaches of shaping materials from bulk.

Methods: A modified Stöber method was used to prepare 30-60 nm monodisperse SiNPs, confirmed by transmission electron microscopy (TEM), through the hydrolysis and nucleation of tetraethyl orthosilicate (TEOS) in an aqueous/organic bilayer. SiNP cores were dye-doped with rhodamine B and regrown to encapsulate fluorophore molecules before being thiolated and subsequently conjugated with DNA via thiol-maleimide crosslinker. Gel electrophoresis was used to visualize DNA attachment by comparing movement of conjugated SiNPs against unconjugated controls.

Results: Crosslinked controls traveled farther in gel electrophoresis than both the SiNP cores and DNA cross-linked SiNPs, which underwent equivalent migration. These results suggest a successful formation of cross-linked DNA with unsuccessful conjugation to the thiolated silica surface.

Conclusion: While the DNA-linker reaction is promising, further research should be conducted in running thiol-maleimide reactions to optimize conditions for SiNP DNA attachment. Successful conjugation will allow for future experiments to proceed in testing DNA-based nanostructures for properties of cell specificity and localization with applications of targeted drug delivery and biosensing.

P14: Inhibition of New Delhi Metallo-Beta-lactamase-1 (NDM-1) by Benzamide Derivatives

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In New Delhi, India 2008, Metallo-Beta-lactamase-1 (NDM-1) was discovered in *Klebsiella pneumoniae* and *Escherichia coli*. NDM-1 catalyzes the hydrolysis of antibiotics that have beta-lactam ring structures, like penicillin. NDM-1 is a subclass B1 meaning it needs one or two zinc ions present to be activated. Furthermore, to inhibit the activity of the NDM-1 zinc binding compounds are being looked at, more specifically benzamide and a benzamide derivative, Chidamide. Chidamide has been known to have a high affinity for class 1 histone deacetylases and has been shown to have manageable toxicity in the body. Chidamide is under clinical trials in Asia and North America. We performed Autodock Vina with Chidamide and benzamide (as a control) for NDM-1 and obtained binding affinities of Chidamide and benzamide -6.9 and -4.4 kcal/mol, respectively. *In vitro* inhibition test was performed, and an IC₅₀ value estimate of 6.15 μM was found. The mode of inhibition was also found to be competitive with a K_i value of 1.60 μM. These observations show that Chidamide may be a potential inhibitor for NDM-1, and further investigations are warranted.

P15: Recombinant expression and purification of membrane proteins; T-cell receptor alpha (TCR α) and Transmembrane serine protease II (TMPRSS2)

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Membrane protein interaction with biomolecules is vital for most cellular functions. They transmit signals between cells and their environment enabling cell recognition and attachment, which are crucial for normal homeostasis. This study aims to express, purify, and characterize two MPs, T-cell receptor alpha (TCR α) and Transmembrane serine protease (TMPRSS2), *in-vitro*. TCR α is a moiety of the T-cell receptor complex that allows antigens bound to the major histocompatibility complex (MHC) to be recognized, thus, vital for cellular immune response. TMPRSS2 is an essential component of the viral infection cascade of the respiratory tracts. It activates the SARS-CoV-2 and the Middle East respiratory coronavirus (MERS-CoV) spike protein, which plays a vital role in host cell entry and is essential for their replication.

A protein consisting of the transmembrane domain of wild-type TCR α was recombinantly expressed in *E. coli* cells. Specific mutations were initiated in the TCR α gene to give four mutants, L14C, K16C, A18C, and M24C. These mutant genes were transformed into competent BL21 (DE3) cells, expressed, and purified using size exclusion chromatography (SEC). Wild-type TCR α was structurally characterized using NMR spectroscopy to determine the dynamics of the side chains. WT TMPRSS2 was similarly expressed and purified. Proteins of interest were identified by SDS-PAGE and LC/MS showing molecular weight bands corresponding to TCR α and TMPRSS2. LC/MS spectra confirmed the TCR α size, and NMR spectra correlate well with the sidechain of WT TCR α . The successful expression, purification and characterization of these MPs are pivotal towards *in vitro* post-translational modification and determining the effect of these modifications on structure and function.

P16: Inhibition of Bla2 by Hydroxamate-containing Compounds

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Metallo-beta-lactamase (MBL) is a growing threat in medical science due to its resistance to beta-lactam antibiotics. *Bla2* is a MBL from the B1 subclass, that came out of the B class of beta-lactamase. Unfortunately, there are no commercial inhibitors available for MBLs. Hydroxamic acid has been shown to chelate with Zn²⁺ ions in previous studies. This study will test nineteen hydroxamate containing compounds against *bla2* to see if inhibition is taking place. Computational analysis was used to determine the binding affinity value for each hydroxamate compound. Since there is not a 3D model of *bla2* available, the closest matching protein to *bla2* had to be used. *Bla2* was isolated and purified from *E. coli*. An enzyme assay was performed to determine if *bla2* was hydrolyzing the beta-lactam ring in nitrocefin. The five best hydroxamate inhibitors were then tested for their inhibition concentration. After successful purification, the enzyme assay showed activity between *bla2* and nitrocefin. IC₅₀ values were determined on each of the five hydroxamate compounds and Scriptaid showed the lowest IC₅₀ value. To conclude Scriptaid, even though come in 3rd on binding affinity, showed the best inhibition concentration value. Scriptaid will be tested on a mode of inhibition to determine if it will show competitive inhibition.

P17: Molecules of Nature: A Summer Academy

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The Molecules of Nature Summer Academy is a residential summer camp sponsored by the Oklahoma State Regents for Higher Education. The camp serves twenty rising eighth and ninth graders from Oklahoma, and was held on the campus of East Central University June 7 through June 11, 2022. During this one-week experience, students conducted a variety of hands-on experiments in the organic laboratory. They also met with University personnel from the recruiting and financial aid office who stressed the importance of planning for college. The primary goals of the Academy is to excite the students about chemistry and to demonstrate to participants that they can thrive while living and learning in a campus environment.

P18: The Impact of Authentic Research-Based Experiences on Students' Learning Outcomes in General Chemistry I Laboratory Course

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The inability of students to draw connections between chemistry principles and daily experiences, as well as other STEM disciplines can hinder their interest in pursuing STEM programs and mastery of interdisciplinary cross-cutting concepts. As gateway courses to many STEM programs, General Chemistry laboratory courses can be revamped to convey interdisciplinary connections increase students' appreciation of science, and improve mastery of cross-disciplinary concepts. In this study, five authentic, inquiry-based interdisciplinary chemistry-biology modules were developed and implemented in the General Chemistry I laboratory course. Some laboratory sections were exposed to the traditional "cookbook" experiments (Comparison group), whereas others were exposed to the interdisciplinary modules (Treatment group). We assessed the impact of the modules on students' cognitive and affective outcomes. This presentation will reveal detailed results centered on students' perceived STEM identity and interdisciplinary chemistry-biology connections in the course as a result of the interdisciplinary curriculum.

P19: Physical and Optical Properties of Biomass Burning Organic Aerosol from Eastern Red Cedar: Hygroscopicity, Absorbance, and Polarity

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Eastern red cedar is a non-native species in Oklahoma that is highly flammable and increases the risk of wildfires across the native tallgrass prairie. It is also a source of biomass burning organic aerosol (BBOA), composed of light absorbing particles, which impact air quality and climate, both regionally and globally. The appearance and composition of eastern red cedar wood varies across the cross section of a tree, so the physical and optical properties of the resulting BBOA may depend on the part of the tree that burns, whether the heartwood, sapwood, or bark. Here, we explore the variations between BBOA generated from the different portions of eastern red cedar. Aerosol samples were generated in the laboratory by smoldering wood samples from the field and collected on quartz filters. The samples were then extracted with either ultrapure water or methanol and used for measurements of UV-vis absorbance. Only the samples that were extracted with the ultrapure water were used for the hygroscopicity measurements, accomplished with a tandem differential mobility analyzer. The solution was diluted and atomized, and then the particles were passed over activated carbon and over silica desiccant. Particles with mobility diameters of 100 nm were then selected and exposed to a known relative humidity, and the size change was monitored. The resulting particle diameter change was used to quantify the water uptake for all three samples, showing that the heartwood had the largest growth out of the three samples. The absorption data showed that the heartwood was the most absorbing in both ultrapure water and methanol, while the sapwood and bark absorbance fluctuates for both solutions in all the spectra that were collected. The absorbance taken in ultrapure water was higher than that taken in the methanol, but the mass absorption coefficient was smaller. These results indicate that the physical and optical properties of BBOA vary for even a single biomass species, depending on the part of the tree that burns, and they provide further insights into the role of eastern red cedar on the tallgrass prairie of Oklahoma.

P20: Sorbent to Fertilizer Technology for Environmentally Friendly Water Treatment

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Water resource pollution due to eutrophication and harmful algal blooms are an increasing concern for the entire planet due to the impact on human and animal health and collapsing aquatic ecosystems. A major contributor to the algal blooms is excess plant nutrients such as nitrogen and phosphate in the water. This nutrient pollution can lead to eutrophication and can become very costly and challenging to manage. We are developing a sorbent in the form of a magnesium-iron layered double hydroxide (LDH) with varying Mg:Fe molar ratios that can capture these plant nutrients and can be employed as a time release fertilizer. The LDHs have the general formula of $[M^{II}_{1-x}M^{III}_x(OH)_2]^{x+} [A^{n-}_{x/n} \cdot mH_2O]^{x-}$, where M^{II} is a divalent cation (magnesium), M^{III} is a trivalent cation (iron), and A^{n-} is an anion. The method used to prepare the LDH involved mixing a low-cost, earth abundant metal salt solution with a solution of sodium hydroxide followed by room temperature aging of the precipitated mixture. Next, the LDHs were isolated by centrifugation and washed extensively with water. The resulting solids were then calcined at 850°C. The phosphate and nitrate uptake capacities of the resulting materials were then measured. The materials were also characterized by attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR), *thermogravimetric analysis* (TGA), microwave plasma-atomic emission spectrometry (MP-AES) and elemental analysis. It was found that a ratio of Mg to Fe in the 1:1 and 2:1 Mg range is the most promising for nutrient uptake.

P21: Biomass Burning Organic Aerosol from Summer and Winter Tallgrasses on the Great Plains: Absorbance, Hygroscopicity, and the Role of Charge-Transfer Complexes

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Biomass burning is the largest source of brown carbon (BrC) aerosol in the atmosphere, where it impacts climate directly by interacting with light and indirectly by interacting with clouds. However, the overall effect that BrC has on climate is not well constrained due to variability in particle composition, evolution, and fate, as well as the possible role of charge-transfer complex formation. Furthermore, these key factors may be dependent on the biomass species. Here, we compare four grasses from the Southern Great Plains in summer and winter, measuring differences in the light absorption and hygroscopicity of the water-soluble portion of the BrC aerosol, to determine the effects of species and season on aerosol properties. BrC generated in the laboratory from grass samples is collected onto filters, then extracted in water. To explore differences in light absorption, the mass absorption coefficients (MAC) of the BrC samples were measured. To test for the presence of intermolecular charge-transfer complexes, the concentration dependence of light absorption was measured. Hygroscopicity measurements were taken by nebulizing dilute solutions of BrC and measuring particle growth as a function of relative humidity, using a tandem differential mobility analyzer. Across seasons, the MAC thus far appears to show that summer samples absorb more light than winter samples at wavelengths of 400-500 nm. Within the same season, only big blue stem differs in MAC when compared to other grasses. Finally, plotting absorbance as a function of concentration in a log-log plot yields a linear dependence with a slope of one for all samples, indicating no intermolecular charge transfer complexes in the bulk solution. Comparing hygroscopicity across seasons and grass type, we find similar growth factors and values of the hygroscopicity parameter, κ . These results indicate the importance of considering seasonality between biomass burning sources and provide further insights into the continuing conversation regarding the contribution of charge-transfer complexes to visible light attenuation in the atmosphere.

P22: Mechanochemical Synthesis of Cyclodextrin-Molybdenum Oxide Nanocomposites

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Mechanochemistry, an approach that uses mechanical forces to induce chemical reactions, presents a promising alternative to the traditional liquid phase reactions. Since mechanochemical reactions usually require very minimal amount of solvent, and even solvent-free conditions, mechanochemical synthesis is viewed as an environmentally-friendly way of doing chemical synthesis. Using a planetary ball mill, we have previously synthesized molybdenum oxide nanoparticles with two distinct morphologies: nanoplates (length: 46.71 ± 20.33 nm, width: 41.55 ± 15.32 nm), and nanowires (length: 300.01 ± 170.60 nm, width: 75.46 ± 15.76 nm). In this study, we explored the one-pot synthesis of MoO₃-β-cyclodextrin nanocomposites using both mechanochemical synthesis and traditional hydrothermal synthesis. We then tested these nanocomposites on their ability to degrade 20 ppm rhodamine B solution, when exposed to blue LED light for 2 hours. Results showed that MoO₃-β-cyclodextrin (hydrothermal) had better removal, $84.3 \pm 3.2\%$, compared to MoO₃-β-cyclodextrin (mechanochemical), and MoO₃ alone, $62.3 \pm 2.7\%$ and $68.0 \pm 1.6\%$, respectively.

P23: Mg²⁺/Al³⁺ Layered Double Hydroxide Synthesis for Phosphate and Nitrate Removal

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Urban runoff and common agricultural practices can produce plant nutrient byproducts, such as phosphates and nitrates, that lead to eutrophication. These plant nutrients accumulate in water systems to spur on algal blooms that can release toxins and contribute to a low dissolved oxygen content in water systems. As a result, eutrophication causes significant damage to wildlife and economic gains. Layered double hydroxides (LDHs) are hydrotalcite materials with proven capabilities in functioning as porous sorbent materials. This study investigates LDHs' capacity to remove phosphate and nitrate plant nutrients from water systems to prevent the environmental harms caused by eutrophication. Materials consisting of a 2:1 ratio of divalent Mg²⁺ and trivalent Al³⁺ were synthesized via a co-precipitation method at varying ratios of sodium carbonate and sodium hydroxide and then calcined to 850 degrees Celsius to determine 1) if materials are capable of removing phosphates and nitrates from concentrated stock solutions of K₂HPO₄ and KNO₃, 2) optimum ratios of Na₂CO₃ and NaOH for removing plant nutrients from aqueous environments, and 3) the chemical make-up of synthesized materials using various characterization methods. Characterization of materials consisted of thermogravimetric analysis (TGA), elemental analysis for total carbon and nitrogen content conducted by Oklahoma State University's Soil, Water, and Forage Analytical Laboratory, microwave-plasma atomic emission spectroscopy, and attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR). Additionally, the best performing sorbent ratios were then calcined to 950 and 1000 degrees Celsius to determine optimization criteria for plant nutrient removal. Results indicate that materials do remove both phosphate and nitrate from stock solutions as indicated by the Hach DR 3900 spectrophotometer analysis and further supported by ATR-FTIR and TGA analysis.

P24: Formation of Hydrogen Peroxide in Commercial Aerosol Generators: Detection, Quantification, and Implications

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Hydroxyl radical plays a central role in the oxidation of organic compounds in the atmosphere, whether in the gas, aqueous, or particulate phases. Hydrogen peroxide is an important source of hydroxyl radical, both in the atmosphere itself and in the laboratory, where atmospheric processes are often investigated under controlled conditions. Recent studies have shown that hydrogen peroxide can form spontaneously in submicron aqueous aerosol particles, an observation that could have profound implications for atmospheric chemistry. Here, we investigate the formation of hydrogen peroxide in two commercial aerosol generators, one for research and the other for pharmaceutical purposes. Submicron aqueous aerosol particles were generated from salt solutions using compressed air, conditioned at a controlled relative humidity, and collected on a custom-built inertial impactor. The resulting droplets were probed with sensitive colorimetric test strips, with a detection range of 0.5 to 25 mg L⁻¹. A colorimetric response from solutions of titanium (IV) oxysulfate, TiOSO₄, which appears yellow upon exposure to hydrogen peroxide, was also explored. For both aerosol generators, droplets produced from ultrapure water and NaCl solutions, without any added chemicals or catalyst, gave positive responses on the test strips, consistent with the earlier observations of spontaneous hydrogen peroxide formation. First estimates of the yield can be determined from the colorimetric response and the volume atomized by the aerosol generator. Importantly, after switching the nebulizing gas from air to ultrapure nitrogen, no response from the test strips was observed. This observation is consistent with recent claims that trace amounts of ozone in air are responsible for the formation of hydrogen peroxide at the interface of submicron particles.

P25: Synthesis, Characterization and Photoluminescent Studies of Two and Three-Coordinate Cu(I) Complexes bearing Diaminocarbene Ligands

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Organic light-emitting diode (OLED) sources are becoming more popular due to their better screen resolution, lower power consumption, and greater versatility as compared to traditional liquid-crystal displays (LCDs).¹ OLEDs typically utilize organic molecules or rare earth metals for their emissive properties, but studies have showed that organometallic complexes can emit wavelengths in the visible region in crystalline and liquid phase at relatively high quantum yields.^{1,2} Sterically hindered N-heterocyclic carbene (NHC) ligands bound to Cu(I) in two- and three-coordinate systems enhance the stability of the photoexcited states by preventing geometrical changes through John-Teller distortion leading to non-radiative decay pathways. Recent studies have shown that copper complexes supported by cyclic amido and diamido carbene ligands are phosphorescent in the visible region in solution phase.² Our group has previously reported heteroleptic Cu complexes bound to imidazole-based NHC and dimethyl-dipyridylamines (dmdpa) ligands to be phosphorescent in solid phase.³ Currently, we are working on the synthesis of copper(I) complexes bearing various six-membered cyclic diamino carbene and carbazole ligands. The mesitylene and diisopropylphenyl derivatives have been synthesized and characterized using x-ray crystallography and are undergoing analysis using UV-Vis and fluorescence spectrometry.

P26: Fourier-Transform Infrared Spectroscopy Study of Asphalt Aging and Its Effect on Chemical Composition

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With over 90% of paved roads in the U.S. being asphalt pavements, their critical role in essential infrastructure is unquestionable. Increased recycling of asphalt concrete from these pavements is an integral component and one of the greatest opportunities for a sustainable infrastructure. Being a core part of the pavement, asphalt is a very complex material. Its composition includes millions of different molecules which vary greatly from one asphalt to the next depending on the source of the petroleum and its processing at the refinery. It has been estimated that asphalt has 10^5 - 10^6 different molecules¹. The explicit representation of exact chemical species present in any asphalt binder is not feasible. One approach has been to capture asphalt chemistry by defining broad categories of molecules. Such an approach relies on generic SARA fractions where the composition includes saturated aliphatic compounds(S), naphthenic aromatics (A), polar aromatics or resins(R) and large polycyclic structures called asphaltenes(A) with heteroatoms. These groups with their different polarities have been related to the colloidal nature of asphalt. Asphalt characterization and design are depending mainly on mechanical and rheological testing, to the near exclusion of chemistry. In this project, we discuss the Fourier-transform infrared (FTIR) spectroscopy study of the asphalt aging and its effect on chemical composition, with a special focus on asphaltene molecules and their O-, N- and S-containing functional groups.

P27: Investigation of the Photophysical Effects of Cysteamine as an Aqueous-phase Ligand for CuInS₂/ZnS Core-Shell Quantum Dots

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The effect of cysteamine on the photophysics of CuInS₂/ZnS core-shell quantum dots was investigated. The core-shell quantum dots were synthesized in the organic phase via the heat-up method. Following synthesis, the native dodecanethiol ligands were exchanged with the polar cysteamine ligands. Ligand exchange was confirmed via phase transfer. Both ensemble measurements and single-particle fluorescent blinking measurements were compared between the organic-soluble and aqueous-soluble quantum dots. The comparison informs of relevant considerations when preparing quantum dots for use in the aqueous phase.

P28: Synthesis and characterization of tri-dentate quinoline-based OCN ligands and their complexes.

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The coordination chemistry of N-heterocyclic carbenes (NHCs) and the application of their transition metal complexes in various fields including catalysis have gained considerable interest over the last few decades. Among different classes of NHC ligands, three-dentate pincer-type systems are particularly important owing to the possibility of chelate formation with metals and readily available positions for electronic and steric modifications. Previously, our group developed some pyridine-based NHC ligands and their Cu(I) complexes, ¹ and examined their application in catalytic C–C and C–X (X = O, N) cross-coupling reactions. ^{2,3} The presence of high-valent Cu–O₂ species was proposed as likely intermediates in the processes, however, the low-stability of Cu(II) species in pincer CNC coordination environment precluded further characterization of these species.

Herein, we report the synthesis and characterization of novel tri-dentate NHC ligands bearing phenol and quinoline wingtips. It has been hypothesized that these quinoline-based OCN ligands have the potential to stabilize higher oxidation states of transition metals including Cu(II). Our current efforts are focused on preparing different derivatives of pincer CNO ligands and investigating their coordination chemistry.

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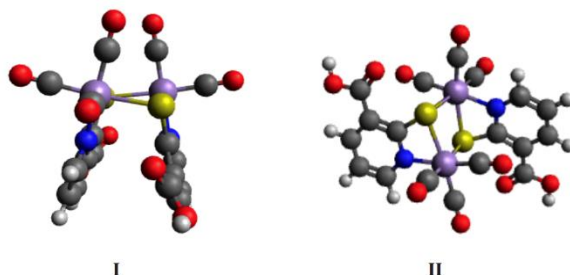
P29: Synthesis, X-ray, and Theoretical Structural Analysis of A Binuclear Manganese Tricarbonyl Thionicotinic Acid Complex

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The reaction of $Mn(CO)_5Br$ with Thionicotinic acid in a 1:1 molar ratio in acetone in the presence $NaBPh_4$ yields selectively only one of the possible two isomers. Repeated experiments show that the isolated products appeared to be cis based on X-ray crystallographic and infrared spectroscopic data. This contrasts with the general belief that a trans-isomer is more stable than cis. To address this issue, we have used density functional theory (DFT) calculations to estimate and compare the energy of formation and thereby the stability of these two geometrical isomers. Specifically, B3LYP (hybrid density functional), TPSSh (meta-hybrid density functional) theory and split valence triple zeta basis set, def2-TZVP, were used for geometry optimization and electronic properties calculations. Results of these DFT calculations suggests that the cis isomeric complex I is energetically more stable than the trans isomeric complex II. The energy differences between cis-complex I and trans-complex II is -2.34 kcal/mole (B3LYP/def2-TZVP) and -3.55 kcal/mole (TPSSh/def2-TZVP). Our results from both the experimental and theoretical studies will be discussed during the presentation.



P30: Nucleophilic attack at the bound NO of cationic group 8 nitrosyl porphyrins

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The interconversion of inorganic-NO_x compounds with their organo-NO_x counterparts plays an important role in the global N-cycle. Heme enzymes and biomolecules are proposed to play key roles in such conversions in the environment. These interconversions may involve the formation of new carbon-nitrogen bonds from their metal-NO precursors. A pathway to such C-N bond formation involves nucleophilic attack at bound NO groups, a process that is well established in coordination chemistry. However, such reactivity in metalloporphyrin bioinorganic chemistry has lagged behind. We previously reported hydride attack at the NO ligand of ferric-NO compounds to yield Fe-HNO derivatives. We previously also demonstrated this nucleophilic attack to other carbon- and nitrogen-based nucleophiles on metalloporphyrin complexes of Fe. For example, aryl anion attack the NO ligand of [(porphyrin)Fe(NO)(L)]BF₄ gives the neutral product (porphyrin)Fe(ArNO)(L), where L is a neutral nitrogenous base. We have extended our investigations into related nucleophilic attacks at the bound NO groups in ruthenium nitrosyl porphyrins of the form [(porphyrin)Ru(NO)(L)]OTf. In our current work, we show that a similar reactivity pattern is present when C-based nucleophiles react with the Ru-NO cation to generate the neutral (porphyrin)Ru(RNO)(L) compounds that are relatively stable in air as solids. Some of these products are isolable in good yields and have been fully characterized by IR and ¹H NMR spectroscopy. We also demonstrate that some N-based nucleophiles react with the bound NO groups to generate new N-N bonds. These and related reactions provide a chemical basis for understanding how heme compounds may be involved in heme-based nitrosations in nature.

P31: Electro-organic synthesis using 3D-printed electrodes

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While a promising field of research, electro-organic synthesis still faces many obstacles before it can be employed on a widespread basis. The use of electricity allows experiments to be carried out in a safer, inexpensive, more controlled way. However, the expensive equipment needed, rigid electrodes used for experiments, and limited reaction area still pose problems for many researchers; 3D printing is an innovative tool that can help alleviate some of these concerns. The ACT-mediated electrochemical oxidation of solketal was used as a proof of concept for the use of 3D-printed electrodes in electro-organic synthesis. Trials were carried out using various electrode types and activation methods to maximize the efficiency of the process. Products were characterized by H-NMR.

P32: Optimization of the Synthesis of Substituted 1,2,4-Triazoles

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Cyclic molecules containing nitrogen, oxygen and sulfur are common in nature, ranging from sugar molecules, over alkaloids to the bases holding together the two strands of our DNA through hydrogen bonding. Many compounds with biological activity used for treatment of common diseases or infections also contain at least one heterocycle in their structure. For example, the antibiotic penicillin has a nitrogen containing heterocycle while the antipsychotic drugs Zyprexa and Seroquel both have sulfur and nitrogen atoms incorporated in their rings. Fluconazole is an antifungal medication which contains two 1,2,4-triazole rings, the topic of the current presentation.

The target of our research is to improve a previous synthesis of substituted 1,2,4-triazoles developed in the Bolliger lab. By using different reaction precursors and developing a different pathway to the desired molecules, we aim to both improve the yields of these reactions as well as make the purification of the products easier. We will compare the outcome of these two alternative synthetic routes and test the new procedure with various amine starting materials.

P33: Adaptation of strain-loadable alkenes for biological uses

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Bioorthogonal chemistry allows further exploration of the intricacy of life through the development of highly selective reactions that occur reliably, even in a complex biological environment¹. Past work in the Weaver group developed a reaction system that utilizes an iridium-based photocatalyst, a cycloalkene, and blue light to transform light energy into molecular strain energy within the cycloalkene². The strained cycloalkene can then conjugate with an azide via a “click” reaction. This reaction is highly selective, fast, and only occurs in the presence of blue light, priming it for use for biological tagging and probing. Both of my aims (*infra vide*) increase the function of this novel reaction system by 1) modifying the cycloalkene to expand its use in biological systems, and 2) further probing of the reaction mechanism, which will allow the technology to reach its full scientific potential. More specifically, I am attempting to modify the structure of the cycloalkenes such that it may be able to conjugate with the azide without photocatalyst. Potential structural candidates were selected based on our hypothesis that the primary hinderance of the direct photochemical reaction is the rate of inter-system crossing was too slow. My second objective is to modify the structure of the cycloalkene such that it can be readily synthesized, conjugated to biological tools easily, and maintain ideal physiochemical properties to be used in biological systems. Continued investigation of this technology is expected to expand our knowledge of this photochemical reaction and refine the technology such that it can be used in diverse applications.

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P34: Amino Acid Exchange in Ni(II) Complexes of Glycine

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Non-canonical α -amino acids continue to play a pivotal role in the advancement of human health and well-being. Unfortunately, access to these materials remains limited. Of the synthetic methods developed for their production the manipulation of Ni(II) complexed glycine imines remains at the forefront. Utilizing this method has allowed for the preparation of sterically constrained glycine derivatives, β -substituted pyroglutamic acids and prolines, as well as optically pure α -amino acids through dynamic resolution of racemic mixtures. Despite the utility of these metal complexes, various aspects have yet to be explored. One such aspect is the potential for amino acid exchange of the metal complex which would open new avenues for the efficient production of optically active non-canonical α -amino acids. Therefore the hypothesis of this project is that the steric demand and electronic nature of the aromatic groups surrounding the imine carbon should effect the exchange rate of the amino acid of the Ni(II) complex. In order to test this hypothesis a series of glycine and phenyl alanine Ni(II) complexes derived from benzophenone, acetophenone, and benzaldehydes which contain various electron withdrawing groups were prepared. The glycine derived complexes were subjected to basic methanolic conditions in the presence of phenylalanine and samples were extracted from the mixture at predetermined times. These samples were processed and analyzed by reversed phase HPLC to determine the ratio of the glycine to phenylalanine complex. This data was used to establish the rate of amino exchange of each complex. In conclusion, the rate of amino acid exchange is accelerated by decreasing the steric demand and introducing electron withdrawing groups. Specifically, the electron withdrawing groups had the greatest effect if they were in a position of resonance with respect to the imine carbon.

P35: Hantzsch Amides for the Selective Reduction of Michael Acceptors

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The main goal of this research study is to develop a new method to selectively reduce electron-deficient alkenes, even in the presence of electron-rich alkenes. For example, the use of a protecting groups could be avoided if the reduction could occur selectively, reducing the number of synthetic steps. In initial studies from our group, we focused on developing a new method for the reduction of Michael acceptors, working primarily with benzyl acrylate. This method is photocatalyzed by Vitamin B12 and 4CzIPN and uses Hantzsch ester as the reducing agent. This method was successful; however, it generated a pyridine byproduct that was difficult to be washed out and separated. In this work, instead of using Hantzsch ester as the reducing agent, we will be examining different amines and Hantzsch amides as reducing agents, as these are expected to be easier to remove after the reaction, simplifying purification. The synthesis of different Hantzsch amides and their ability to act as reducing agents for the reduction of benzyl acrylate will be discussed.

P36: Broadening the Boundaries of Friedel-Crafts: Access to 1,1-diarylcyclohexyl motifs through visible light photocatalysis

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Aromatic heterocycles and carbocycles are ubiquitous features of biologically active molecules. The installation of such motifs is of great importance to drug and agrichemical synthesis. One common strategy for the installation of such groups is the Friedel-Crafts benzylation reaction. Traditional Friedel-Crafts reactions are plagued by the harsh reaction conditions (high acidity, intense heat) required to carry out the necessary electrophilic aromatic substitution. These conditions greatly limit the scope and stage of synthesis at which aromatic structures can be introduced. Here we present a surrogate reaction which utilizes visible light, a highly efficient iridium photocatalyst, and mild reaction conditions to produce pharmacologically relevant and difficult to access 1,1-diarylcyclohexyl quaternary carbon centers.

P37: Access to Tricyclic Heteroarenes by an Iodine-promoted Cyclization Reaction

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For many years, investigations on nitrogenous heterocycles have been an essential part of organic chemistry due to their widespread use in medications and functional materials. Our research examines alternative ways to prepare nitrogen-containing heteroarenes while also minimizing the formation of unwanted by-products. Many of our target molecules have structural similarities with biologically active compounds used for a variety of conditions, such as cancer, anxiety, and fungal infections. Starting by optimizing a preliminary procedure from the Bolliger lab, we were able to improve the isolated yields for the iodine-promoted cyclization step. In this presentation, we will show the results of our substrate scope and discuss possible reaction mechanisms. Ultimately, we hope that our research will pave the pathway to novel species with biologically relevant functional groups.

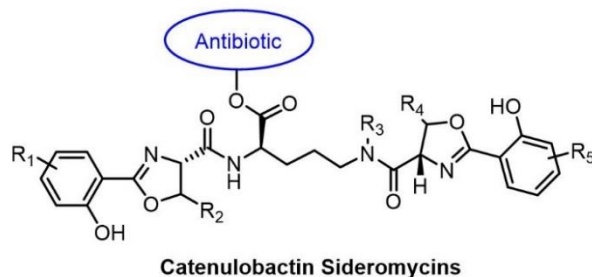
P38: Efforts Toward Synthesis of Sideromycins with Catenulobactin B to Improve Antibiotic Penetration into Gram-Negative Bacteria

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Gram-negative bacteria are resistant to many antibiotics currently available on the market. Given the fact that some of the Gram-negative bacteria are amongst the most virulent bacteria, more methods are required to combat their infections. The presence of the highly selective outer membrane in their cell walls made of lipopolysaccharides makes most of the antibiotics that are active toward Gram-positive bacteria to be inactive toward Gram-negative bacteria. To overcome this problem and improve the ability of antibiotics to penetrate Gram-negative bacterial cell walls, designing sideromycins using a novel siderophore named catenuobactin B is underway. Siderophores (molecules that transport iron into bacteria) are conjugated with antibiotics to form sideromycins. It is envisioned that the synthesis of these novel sideromycins will help the antibiotics to circumvent the porin-mediated small molecule transportation and penetrate the Gram-negative bacterial cell walls through active transportation. Total synthesis of catenuobactin B is underway as the first step in this endeavor utilizing commercially available amino acids and other simple compounds. Once the total synthesis of this natural product, as well as its analogs, is accomplished, a library of sideromycins is proposed to be populated to screen their ability to penetrate Gram-negative bacteria.



P39: Access to substituted tricyclic heteroarenes by an oxidative cyclization reaction

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Heterocycles are a structural feature found in many active pharmaceutical ingredients. Among these biologically active compounds are sulfur-containing heteroarenes of which some have demonstrated activity against fungal infections, inflammation, or cancer. In this presentation we will show the newest results of the Bolliger group's approach to the synthesis of fused heterocycles. We have prepared a wide range of substituted starting materials which allow us to study the scope of this oxidative cyclization reaction. We discovered that in a one-pot two-step procedure we can selectively deprotect the thiol in the presence of a variety of different functional groups and subsequently convert it to the tricyclic heteroarene upon addition of an oxidizing agent. We will present the results obtained with substrates containing electron-donating and electron-withdrawing substituents as well as the conclusions drawn thereof in terms of the reaction mechanism.

P40: Lutidine enabled Photocatalytic Giese type reactions of alkyl/aryl halides

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The use of photocatalysis to generate radicals in a controlled fashion has become an important synthetic strategy in recent times. The reducibility of alkyl halides prevented their broader implementation in a radical generation. Previously, katriisky and collidinium salts have been demonstrated as excellent alkyl radical precursors when combined with photocatalysis. Herein we explore using enhanced nucleophiles like lutidine over substituted pyridines like collidine to replace halides and capture the electron to normalize the variable redox potentials. The increased nucleophilicity of lutidine allows for the possibility of nucleophilic co-catalysis which was not previously possible. Lutidine also facilitates the salts to be made in situ as opposed to premade salts.

P41: 3D Printed Electrodes and Devices for Electro-Organic Synthesis

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3D printing is a rapid prototyping technique that has recently been employed in electrochemistry, both as electrochemical cells and, more recently, as electrode materials. In this project, unique electrode geometries and electrochemical cells were designed, printed, and tested for the specific application of electro-organic synthesis. We have evaluated the relationship between the effective surface area of the 3D printed electrode on its electrochemical performance. Additionally, new 3D printed devices for the activation of the 3D printed electrodes were designed to enable activation of larger electrodes.

P42: Probing electronic and hydrodynamic properties of fluorescent probe molecules in reverse micellar environment

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The electronic and hydrodynamic properties of fluorescent texas red dyes have been investigated in confined and crowded reverse micellar environments. Various steady-state spectroscopic techniques such as UV-Vis absorption and fluorescence emission as well as Dynamic Light Scattering (DLS) were employed to determine various photophysical parameters such as band shift and fluorescence quenching etc. The results obtained in confined environments were compared with the results in aqueous environments. Our experimental observation shows that texas red behaves very differently in reverse micellar environment as compared to aqueous environment. Furthermore, our results show that the dye undergoes aggregation inside reverse micelles.

P43: Photophysical and hydrodynamic properties of Alexa Fluoro (AF) 647 dyes in confined reverse micellar environment in presence of Graphene Oxide nanoparticle

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The photophysical and hydrodynamic properties of fluorescent Alexa Fluoro (AF 647) dyes have been investigated in confined and crowded reverse micellar environments in presence of Graphene Oxide nanocolloid (GONc). Various steady-state spectroscopic techniques such as UV-Vis absorption, fluorescence emission and excitation were employed to unravel the photo physics of the probe molecules. The results obtained in confined environments were compared with the results of the aqueous environments. Our results show that AF 647 dye behaves very differently in reverse micellar environment as compared to aqueous environment. Furthermore. Our findings show that AF 647 undergoes dimerization in the smallest size of the revers micelles. Finally, our observations have provided us the necessary protocol to use AF 647 as a dye label to investigate protein folding in reverse micellar environment.

P44: 19 K Argon Matrix Isolated 5-Fluoro-2'-Deoxyuridine Analyzed by Vibrational Spectroscopy and Supercomputer Calculations using GAMESS

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5-fluoro-2'-deoxyuridine, sometimes called Floxuridine or Calbiochem, is an experimental anticancer agent shown to have activity against a variety of malignant neoplasms, including mouse mammary tumors and colorectal carcinomas. Floxuridine acts as an inhibitor of the S-phase of cell division by acting as a pyrimidine analog. This selectively kills rapidly dividing cells. This poster presents the 19 K frozen argon matrix isolated FTIR spectrum of Floxuridine containing multiple functional groups with extensive potential for intramolecular hydrogen bonding. Our results present the frozen argon matrix isolated monomer spectrum of Floxuridine which gives a pseudo ideal gas phase type spectrum with little if any intramolecular hydrogen bonding. This greatly facilitates the comparison of the experimental FTIR spectrum with LCAO-MO *ab initio* density functional computed infrared spectrums. SQM scaled LCAO-MO computational Hessian studies at the B3LYP/6-311G(d,p)++ and other theoretical levels are underway to understand the structure and possible conformers of this pharmaceutical and to identify the vibrational assignments using FCART 7.0 (Pulay SQM Scaling) and GAMESS (*ab initio* MO program) using our HP (6000 core) super-computer Titan.

P45: Study of Electronic Properties of Pi-electron Systems Containing Silicon-Silicon Double Bonds Using Density Functional Theory

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The Silicon atom is located below the carbon atom in Group IVA in the periodic table. Although both elements are in the same group in the periodic table, both elements possess some significant distinct properties. Carbon is a central element in organic compounds, and silicon is the critical element of inorganic compounds. Although compounds with carbon-carbon double and triple bonds are ubiquitous, compounds with silicon-silicon double and triple bonds are very limited due to their instability. Recently, several groups have successfully prepared compounds containing silicon-silicon double and triple bonds. However, the progress of silicon-silicon double and triple bond compounds are still in the preliminary stages. We are trying to theoretically understand the electronic properties of compounds containing silicon-silicon double bonds using density functional theories (DFT). In this meeting, we will present the electronic properties of silicon-silicon double bonds concerning the electron-withdrawing and electron-releasing substitute groups.

P46: FTIR Spectroscopy of Ethyl 6-Methyl-4-Phenyl-2-Sulfanylidene-1,2,3,4-Tetrahydro-Pyrimidine-5-Carboxylate Matrix Isolated in 18 K Frozen Argon

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Ethyl 6-Methyl-4-Phenyl-2-sulfanylidene-1,2,3,4-tetrahydro-Pyrimidine-5-Carboxylate (EtPSPc) is the sulfur analog of the Biginelli reaction product Ethyl 6-Methyl-4-Phenyl-2-oxo-1,2,3,4-tetrahydro-Pyrimidine-5-Carboxylate. Biginelli reaction products are serious candidates for combinatorial studies of compounds useful for a variety of pharmaceutical purposes. This poster presents the 18 K frozen argon matrix isolated FTIR spectrum of EtPSPc. EtPSPc contains multiple functional groups with extensive potential for intramolecular hydrogen bonding. Our results present the frozen argon matrix isolated monomer spectrum of EtPSPc which gives a pseudo ideal gas phase type spectrum with little if any intramolecular hydrogen bonding. This greatly facilitates the comparison of the experimental FTIR spectrum with LCAO-MO *ab initio* density functional computed infrared spectra. SQM scaled LCAO-MO computational Hessian studies at the B3LYP/6-311G(d,p)++ and other theoretical levels are underway to understand the structure and possible conformers of this pharmaceutical and to identify the vibrational assignments using FCART 7.0 (Pulay SQM Scaling) and GAMESS (*ab initio* MO program) using our HP (1200 core) super-computer Titan.