

Programming Booklet:

ACS Midland Fall Scientific Meeting 2023

November 3, 2023
Central Michigan University, Mt. Pleasant MI

**Additional meeting details, including parking and directions
can be found at:**

<https://midlandfsm.org/>

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2023 Fall Scientific Meeting Schedule

FRIDAY November 3, 2023

Time	Location	Event	Details
11 AM - 6 PM	BIOSCI - Atrium	Registration	
12:00 - 12:50 PM	BIOSCI - 1010	Meeting welcome & Keynote address	“Infrared Spectrometry: An Entrepreneur’s Journey” Martin Spartz
1:00 - 2:25 PM	BIOSCI - 1015	Materials Speed Presentations	1:00-1:50
		Oral Presentation, Materials Track	1:55-2:25 - Megan Thomas
	DOW - 135	Analytical/Biochem Speed Presentations	1:00-2:25
2:30 – 3:00 PM	BIOSCI - Atrium	Coffee Break	
3:00 - 4:40 PM	BIOSCI - 1010	Oral Presentations, Analytical/Biochem Track	3:00-3:30 – Nicole Shriner
			3:30-4:00 – Hyder Aliyar
			4:00-4:20 -Koudi Zhou
			4:20-4:40 – Mary Beth Seasholtz
	BIOSCI - 1015	Oral Presentations, Materials Track	3:00-3:30 – Chris Nelson
			3:30-4:00 – Aliakbar Yazdan 4:00-4:20 -Koksal Karakus
4:40 - 6:00 PM	BIOSC - Atrium	Poster Session w/ food & drink	
6:00 – 8:00 PM	The Cabin	Networking, Pizza, and beverages SPONSORED by Midland Section ACS-YCC	

SATURDAY November 4, 2024

Time	Location	Event
9:15 AM – 12:00 PM	BIOSCI - Atrium	Registration
10 AM – 12:00 PM	BIOSCI - 1015	Careers & Vendors Open House
10 AM – 12:00 PM	BIOSCI - Atrium	Volunteering w/ Midland Local ACS
12:00 – 2:00 PM	Hunters Ale House - Cask Room	Lunch & Brewery Tour

Keynote Presentation



Infrared Spectrometry: An Entrepreneur's Journey from Technology to Start-up to Fortune 500

Martin L. Spartz Ph.D.

Analytical Chemist / Spectroscopist - Retired

Email | martyspartz@gmail.com

Martin Spartz | 2023 Midland Local Section Fall Scientific Meeting

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12:00-12:50 pm, BIOSCI 1010



Infrared spectroscopy has been used as a qualitative analytical tool for more than 80 years. FTIR spectrometers have been widely used since the 1980s due to their speed, improved signal-to-noise and their resolution and frequency precision.

When FTIR spectrometers are applied to gas or vapor phase samples at controlled temperature and pressures, the resulting spectra can be both highly qualitative and quantitative due to the reproducibility of the infrared absorption spectrum. Each spectrum is so consistent that a calibration spectrum generated on one instrument can be used forever on that instrument and be easily transferred to any similar instrument. Unlike mass spectrometers and other gas detection systems, the analyzer (spectrometer / source / detector) does not interact with the sample (a beam of light is passed through the sample), so the calibration spectra once generated can be utilized for the life of the instrument.

Over the last six years, Max Analytical Technologies, now a part of Thermo Fisher Scientific, made two major breakthrough discoveries along with many smaller discoveries that added new levels of sensitivity to FTIR gas analyzers and their applicability to chromatography. First, we discovered a new way to couple FTIRs to gas chromatographs that allow quantitative calibration spectra to be transferred from instrument-to-instrument with more than 9 orders of linear dynamic range and not require liquid nitrogen-cooled MCT detectors. While doing so, we also developed analysis algorithms that do not require prior knowledge of the sample matrix or complete chromatographic separation to achieve

accurate quantitative results for the required analytes. Although the current technology is not as sensitive as commercial GC-MS analyzers, it could be an ideal technology for process labs where both quantitative and qualitative information is required.

A second major discovery relates to improving the sensitivity of FTIR gas analyzers by nearly 2 orders of magnitude. Before this discovery, commercial FTIR gas analyzers with 5 to 10 m gas cells could measure gases down to the 1 – 10 ppbv range. With the development of StarBoost™, or what is now in the industry being called Optically Enhanced FTIR (OE-FTIR), we have been able to achieve measurements in the 10 – 50 parts-per-trillion range. The spectra collected at these levels can have < 1 micro absorbance baseline noise. To effectively use this new level of sensitivity other methods also had to be developed to reduce or eliminate baseline drift and spectral interferences so they do not affect the quantitative measurement. FTIR gas analyzers can have 0.01 to 0.10 absorbance baseline drift over time or 10,000 to 100,000 greater than the achievable baseline noise and analyte peak signal.

These discoveries and a brief history of the author will be provided during this presentation.

Invited Presentations

Case Study for Developing Sustainable Materials: Froth-Pak™ Spray Foams

Megan M. Thomas
DuPont, Midland MI 48642

1:55-2:25 pm, BIOSCI 1015

Buildings account for roughly 40% of global greenhouse gas emissions and DuPont is committed to developing products that enable the reduction of both embodied and operational carbon. DuPont's Froth-Pak™ branded low pressure, two-component spray polyurethane foam products are used to seal and insulate various spaces within the building envelope. These products have undergone a transition out of high global warming potential (GWP) blowing agents. The new innovative blowing agent solution for Froth Pak™ Spray Foams has shown to be a promising and stable solution, maintaining superior air sealing and insulating properties while offering a significant reduction in greenhouse gas emissions (GHG). By formulating Froth-Pak™ Spray Foams with the new liquid HFO-1233zd and CO₂, DuPont has decreased the GWP of the blowing agent used in the product to near zero.



Bio: Megan Thomas received her Ph.D. in Organic Chemistry at Northwestern University in 2012 after obtaining her Bachelors of Science from Saint Mary's College Notre Dame in Chemistry and Mathematics. She joined The Dow Chemical Company as a chemist in Dow Building Solutions in 2012 and transitioned with the business to DuPont in 2019. Her focus is on developing and improving sustainable one- and two- component polyurethane foam products. She was the leading chemist on the development and transition of our Froth-Pak™, Tile Bond™, and Insta Stik™ polyurethane products to lower global warming potential formulations – work that has gained recognition for DuPont through several awards. In her spare time, Megan likes to hike, climb, write, and ride horses, and she tries to drag her lovely children along when possible.

Spray Deposition: Quantifying and reducing splashing and bouncing of droplets on leaf surface mimics

Christopher W. Nelson¹, Michael Tate², Heather Wiles¹, Matt Crimmins¹, Carol Mohler¹

¹Core R&D - Formulation & Materials Science, Dow Inc, Midland MI

²Dow Industrial Solutions, Dow Inc, Midland MI

3:00-3:30 pm, BIOSCI 1015

The efficiency and effectiveness of spray-applied agricultural products is strongly influenced by their deposition performance. Improving the retention of fluid on the leaf surface reduces cost, eliminates waste, and mitigates undesirable overspray. The physics of deposition are complex and include phenomena such as droplet impact, expansion, retraction, and splashing. These effects ultimately depend on the interplay of the material properties of the fluid, surface properties of the leaf, and the properties of the in-flight droplet. Here, we review the development and application of a multi-step workflow for characterizing the deposition performance of polymeric additives. Special emphasis is given to the way in which this complex and open-ended problem is approached and solved in the context of industrial R&D.



Bio: Chris Nelson is a Research Scientist in Core R&D at Dow. Since joining in 2016, Chris has led a number of projects in the areas of interfacial and colloid science, including surfactant performance, phase behavior, drop dynamics, and microfluidics. This work was aligned to a variety of different Dow businesses and applications, ranging from the stability of sunscreen to the retention of droplets on leaves. Prior to joining Dow, Chris earned his Ph.D. in Mechanical Engineering from Carnegie Mellon University under the advisement of Professor Shelley Anna, where he worked to develop small-scale fluid manipulation techniques to study colloidal and interfacial phenomena.

New frontiers and applications in biochemical and analytical chemistry

Nicole Shriner

Dept. Chemical Engineering & Materials Science, Michigan State University, East Lansing MI

3:00-3:30 pm, BIOSCI 1010

Corn is the most widely used cereal grain in whiskey products as most grain bills (recipes) are at least 51% corn, with some being as much as 100% corn. Unfortunately, not all corn is created equal. Corn can vary like any other crop in the color, composition and flavor among other attributes. There are many, many varieties of corn that are grown throughout Michigan and the United States. Most varieties are chosen based on yield and extract content, among agronomic variables that lead a farmer to choose to grow and sell a specific variety at their farm. This selection process has resulted in nearly all of the corn produced from hybrid #2 yellow dent varieties, for which a surprisingly low amount of variation exists between varieties. More broadly, corn varieties exhibit a wide range of characteristics, particularly those varieties that are open-pollinated instead of hybridized. I will discuss the on-going research that I am part of which explores the wider range of corn and rye genotypes. We have seen that varieties have different flavor profiles and aging potential. The data has and will give distillers the ability to find unique flavors in corn and rye, as well as marketing potential that comes with utilizing varieties that are heirloom and have other unique properties. I will also discuss the popular conversation around grain terroir which suggests that the same varieties of grain grown in different regions of the world will make inherently different types of whiskies.



Bio: Nicole Shriner is a Teaching Specialist in the Department of Chemical Engineering and Materials Science. She received her BS in Chemical Engineering in 2014 at Michigan State University with concentrations in biomedical engineering and fermented beverage science and technology. She completed her PhD in Chemical Engineering at Michigan State University in 2018. Her dissertation was titled 'Cyclic Distillation for Energy Conversion in Distilled Spirit Production.' She completed a Master Brewer degree from the World Brewing Academy at Siebel Institute of Technology in Chicago, Illinois and Doemen's Academy in Munich, Germany in July 2019. Nicole has compiled a total of 10 years of experience working at, or with, distilleries, breweries and wineries. She manages the fermented beverage analysis lab at Michigan State through which she completes analyses and facilitates research with industry members from raw materials to final fermented beverage product. Nicole collaborates with members of the College of Natural Science and MSU extension on research related to hops, cereal grain and fruits for fermented beverage production.

Research topics include: use of milk permeate by-product stream from the Michigan Milk Producers Association to produce food grade ethanol (vodka) via *K. Marxianus*, diacetyl production, reduction and control in beers brewed with raspberries and other adjunct sugar.

Role of silicone and acrylic pressure sensitive adhesive technologies on the transdermal drug delivery of diclofenac base

Hyder Aliyar
DuPont, Midland MI 48642

3:30-4:00 pm, BIOSCI 1010

Transdermal administration of a non-steroidal anti-inflammatory drug (NSAID) is highly recommended over oral intake for chronic conditions like arthritis pain. Delivering the right amount of drug in a sustainable fashion for an extended time using a more patient-compliant dosage form is strongly desired. Being a primary constituent in the modern matrix-type transdermal skin patch formulations, the pressure sensitive adhesive (PSA) technologies play a key role not only in the patch adhesion to the skin but also in the delivery of drug. PSA technologies typically used include polyisobutene, acrylic and silicone. While individual PSA may fulfil the needs sporadically in patch formulations, the advantage of using a blend of PSA technologies has been demonstrated in this study to deliver a model drug diclofenac base (DCF) efficiently. With other variables kept constant including [DCF] at 2%, a patch formulation made using acrylic PSA delivered about 54 μg , a patch formulation made using silicone PSA delivered about 96 μg , whereas a patch made using a blend of acrylic and silicone PSA delivered about 122 μg . The result was obtained when patches were tested in-vitro for DCF permeability through human cadaver epidermis for 48 hr at 32°C. The right ratio of PSA blends in the patch formulations also showed the possibility of attaining higher DCF delivery rate than that by patch formulation containing acrylic PSA or acrylic-rich PSA blends. The patch formulations containing PSA blend was also found performing best in terms of patch adhesion and DCF's solubility in the patch.



Bio: Hyder is working as a Lead Scientist in the Medical Silicones, Healthcare business unit of Electronics and Industrial division of DuPont. At work, his focus is to investigate and evaluate silicone and silicone-organic hybrid technologies for topical, transdermal drug delivery and skin care product development. He has a PhD in Polymer Science from University of Madras, India. For the last 20+ years, he has gained research and product development experience, all almost on polymeric materials for medical device and drug delivery, via working in research institutes, universities and industry in India, Japan and here in US. Prior to DuPont, he was at Dow Corning and subsequently at Dow.

Contributed Presentations

Metal-Sulfur Batteries: Opportunities and Challenges

Aliakbar Yazdan

Central Michigan University, Mount Pleasant, 48859

3:30-4:00 pm, BIOSCI 1015

Metal-sulfur batteries, including lithium-sulfur batteries, have attracted significant attention as promising energy storage systems. However, the presence of the polysulfide shuttle effect poses a major challenge, which leads to poor cycling stability and limited capacity retention. This research focuses on the exploration of novel strategies to overcome this issue and improve the performance of metal-sulfur batteries.



Bio: Al Yazdani is a chemical engineer with a Ph.D. from Ohio University, specializing in electrochemistry and lithium batteries. He worked as a postdoc at Texas Tech University, focusing on electrocatalysts and their versatile applications, and subsequently as a Battery Material Scientist at Ampcera Inc., where he specialized in solid-state batteries and various cathode and anode materials. Currently, he is a Postdoctoral Researcher at Central Michigan University, dedicated to resolving challenges in metal-sulfur batteries, particularly addressing issues with lithium-sulfur batteries.

Modeling the density profile of a supported thin film using nonlinear partial differential equations

Koksal Karakus

Central Michigan University, Mount Pleasant, 48859

4:00-4:20 pm, BIOSCI 1015

In our study we are modeling the density profile of a supported liquid thin film (glycerol on silica), which was originally simulated by Cheng et al. (Journal of Chemical Physics 143, 194704 (2015)) using classical Molecular Dynamics. We initially represent this profile as a stationary solution of a nonlinear partial differential equation (PDE). The density profile at the free (air) surface and the middle region of the film is well-described by a kink solution of the sine-Gordon equation (SGE). To account for the density oscillations near the silica surface, we have added a term proportional to the fourth-order spatial derivative to the original SGE, which is needed to capture the influence of the crystalline structure of the silica substrate on the adjacent glycerol layers. Having the functional form and coefficients of our PDE, we can proceed to construct an appropriate density functional theory (DFT) for which the density profile emerges as the local or global free energy minimum. A possible further study should include completing the formulation of our DFT, investigating the stability of its one-dimensional solutions against various perturbations, and exploring non-stationary, time-dependent solutions.

Parts per Billion of Nitrite in Microcrystalline Cellulose by Ion Chromatography Mass Spectrometry with Isotope Labeled Internal Standard

Koudi Zhou

IFF/Pharma Solutions, Midland MI 48640

4:00-4:20 pm, BIOSCI 1010

Regulatory authorities like the U.S. Food and Drug Administration (FDA) have set strict specification levels for N-nitrosamines in finished drug products. Nitrite is a potential precursor for the formation of probable carcinogenic N-nitrosamines when secondary or tertiary amines are also present in the active pharmaceutical ingredient (API) synthesis or drug formulation process. An accurate and sensitive determination of nitrite will be useful when a drug product manufacturer chooses to investigate the reaction kinetics between nitrite and amines or to select appropriate excipients for its drug formulation. Pharmaceutical excipient manufacturers may also need an accurate nitrite measurement to investigate the nitrite content in their excipients. This study details the development and validation of an ion chromatography mass spectrometry (IC-MS) method for trace nitrite determination in microcrystalline cellulose materials, one of the important pharmaceutical excipients used in many drug formulations. MS operated under selected ion monitoring mode was used to solve the commonly encountered interference issue with conductivity detection, and nitrite isotope internal standard was employed to address the ion suppression issue with MS detection. The installation of an after-column “jumper” to flush water with an auxiliary pump through the MS when it is not used for data collection avoided sensitivity loss due to trace salt accumulation in the ion source. Validation of the optimized method was satisfactory with linearity, precision, and recovery. The limit of detection and limit of quantitation were 0.005 and 0.016 ppm, respectively.

Lessons Learned over 30 Years of Applying Chemometrics in the Chemical Industry

Mary Beth Seasholtz
Retired from Dow, Inc.
mbseasholtz@outlook.com

4:20-4:40 pm, BIOSCI 1010



This presentation will review lessons learned over a 30-year career using chemometrics within the chemical manufacturing industry. Questions such as 'How is chemometrics used to make money?' and 'What are the challenges?' will be addressed.

Poster Presentations & Abstracts

Thematic Legend:

Education & Outreach	Analytical	Biochem	Materials
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Poster Number	Presenter	Title	Affiliation
1	Wendell Dilling	ACS Awards Won by the Midland Section for Outstanding Performance by a Local Section	Central Michigan University
2	David Baker	Integrating Authentic Research Experience into Organic Chemistry Laboratory Course	Delta College, University Center, 48710
3	Cassie Gardyszewski	An Evaluation of an Organic-Based Lab Experience in General Chemistry	Central Michigan University
4	Nathan Alchin	Synthesis and Characterization of Iron Single Atom Catalysts	Central Michigan University
5	Derek Schoch	Do Bees Dine with Their Neighbors? Analysis of Bee Pollen by Light Microscopy	Project Seed MSU St. Andrews
6	Brendan Pihaylic	Analysis of Beer Antioxidants and the Aging of Beer	Central Michigan University
7	Tristan Mosher	Investigation Into the Link Between Fecal Contamination and Waterbody Qualities	Saginaw Valley State University
8	Konika Konika	Total syntheses of Aspidostomides D, E and F via unprecedented Strecker reaction on Indole	Michigan State University
9	Nanzhu Li	SYNTHESIS OF METHYL GALLATE-BASED GENERATION 2 ANTIOXIDANT DENDRONS	Central Michigan University
10	Warren Jacobs	Determination of the Efficacy of Biochar in Removing Antibiotics from Aqueous Solution	Saginaw Valley State University
11	Alexis Glumm	Synthesis, characterization, and electrochemical analysis of synthetic biomolecule models containing ruthenium with hydroxamate and/or nitrosyl ligands	Saginaw Valley State University
12	Devon Schultz	Actin Interactions with the Actin Crosslinking Domain of MARTX from <i>Vibrio cholerae</i>	Central Michigan University
13	Regan Kopesky	RNAi Screen for RNA binding proteins that enhance microRNA activity after dauer diapause in <i>C. elegans</i> .	Central Michigan University
14	Kaylee Taylor	Developing and Optimizing Bioluminescent Neurotransmitter Sensors and Neuromodulators	Central Michigan University

15	Emma Doederlein	Progress toward developing a catalytically inactive hydrolase to selectively detect Mycobacterium tuberculosis	Central Michigan University
16	Yashpal Singh	Analyzing Perdew-Zunger Self-Interaction Corrections for Reaction Barrier Heights with Semi-Local Density Functionals: Unraveling the Evolution of Stretched Bond Errors	Central Michigan University
17	Jaden McLaury	Antimicrobial properties of a diphenyl beta-lactone	Saginaw Valley State University
18	Michael	Bioluminescent Kinase Sensors for detection of growth factor signaling in U87 glioblastoma cells.	Central Michigan University
19	Kingsley AGU	Design and Synthesis of Mycolic Acid Probes to Investigate the Mycobacterial Outer Membrane	Central Michigan University
20	Arjun Poudel	Systemic Delivery of G4 PAMAM Dendrimers-Progesterone complex Intraperitoneally in MCAo Rat Models	Central Michigan University
21	Emily Maskill	Synthesis and characterization of trehalose-biotin conjugates as tools for the detection of mycobacteria	Central Michigan University
22	Evan Siemienkiewicz	Screening Trehalose Synthase Variants for Substrate Tolerance with Trehalose Analogs for the Inhibition of Mycobacterium tuberculosis.	Central Michigan University
23	Hiruni Kamali Pallage	Enhancing Biochemical Insights Within the Brain via Q-ball Imaging	Central Michigan University
24	Priscilla Dzigba	Host-directed immune targeting of mycobacteria through cell surface glycan engineering	Central Michigan University
25	Blessed Agbemade	SYNTHESIS OF CARNOSINE-BASED AQUEOUS-SOLUBLE ANTIOXIDANT DENDRIMERS FOR BIOMEDICAL APPLICATIONS	Central Michigan University
26	Karishma	Targeting Mycobacterium tuberculosis persistence through inhibition of the trehalose catalytic shift	Central Michigan University
27	Ashley Slaviero	An in-silico pipeline for the rational directed evolution of light-sensitive transcription factor EL222	Central Michigan University
28	Ulysses Johnson	Development of degradation-resistant trehalose analogues: leads for treatment of cardiometabolic disease and inhibition of microbial pathogens	Central Michigan University
29	Swati Singh	Pectin-Stabilized Gold Nanoparticles: An Insight Mechanism of Targeted Drug Delivery	NanoSynthons LLC
30	Evelyn Wang	NIR-assisted stereolithography for high performance polymer derived ceramic	Michigan State University

31	Catriana Nichols	Removal of Arsenate and Ammonia from Water by Adsorptive Membranes and Resins	Waste Water Filtration Polymers / Central Michigan University
32	Mayson Whipple	Facile Route for Polyether Bioconjugation via a Functional Hydroxysuccinimidyl Ester Initiator	Michigan State University
33	Emily England	Evaluation of Stress-Strain and Fracture Behavior in Patterned Hydrogels	Michigan State University
34	Mayank Singh	PEGylated Poly(amidoamine) Dendrimers Toward Translational Nanotherapeutics	NanoSynthons LLC
35	Isaac McWethy	Impact of Templating Agent on the Photocatalytic Activity of Iron-Doped Graphitic Carbon Nitride	Central Michigan University
36	Denghao Fu	Characterization of network heterogeneity in polymerized dental adhesives	Michigan State University
37	Jacquelyn Sundstrom	Substrate-Free Polymer-Ceramic Nanocomposites for Energy Applications	Central Michigan University
38	Sabrina Curley	Chemically and Physically Patterned Polymer Surfaces of Photopolymerization Induced Phase Separating Resins Using Interfacial Interactions to Guide Surface Morphology	Michigan State University
39	Allie VanZanten	Investigating Instability Behaviors to Understand the Relaxation Dynamics of PEG Hydrogels	Michigan State University
40	Quinn VanZile	Synthesis of Organic Compounds for Sustainable Energy	Project SEED- MSU St. Andrews
41	Itzel Marquez	Synthesis of graphitic carbon nitride functionalized with imprinted polymers for the removal of arsenate and ammonia in water	Project SEED
42	Paige Bricault	Dental Adhesives	Central Michigan University
43	Shubhan Nagarkar	Utilization of Additive Manufacturing for Biopolymer (PCL and PLA) Scaffolds in Facilitating Trabecular Bone Osteogenesis	MSU St. Andrews

1. ACS Awards Won by the Midland Section for Outstanding Performance by a Local Section

Wendell L. Dilling and Dale J. LeCaptain

Department of Chemistry and Biochemistry
Central Michigan University, Mt. Pleasant, Michigan

The Midland ACS Section has won 28 Outstanding Performance by a Local Section Awards, 50% of the awards available to a single section, since the program began in 1968. These awards recognize sections that have demonstrated excellent overall achievement by offering multiple programs for members and reaching out to their communities. Sections are grouped according to size from small to very large. One award was given in each of the six size categories. The table shows the Section chairs in the years the Outstanding Performance was won except the first two where the awards were won the following year. Many award plaques and trophies will be shown.

	Year	Midland Section Chair
1	1973	Donald R. Petersen
2	1990	William C. Pike
3	1991	M. Peter Dreyfuss
4	1992	Vicky S. Cobb
5	1993	Gretchen S. Kohl
6	1994	Robert E. Kohrman
7	1999	Debora F. Bergstrom
8	2000	Wendell L. Dilling
9	2001	George W. Eastland, Jr.
10	2003	Michael J. Owen
11	2005	Patrick B. Smith
12	2006	Buford Lemon
13	2007	Dee A. Strand
14	2008	Dorie Yontz
15	2010	John D. Blizzard
16	2011	J. Patrick Cannady
17	2012	Regina M. Malczewski
18	2013	Wayde V. Konze
19	2014	Michelle R. Cummings
20	2015	Regina M. Malczewski
21	2016	Jaime Curtis-Fisk
22	2017	Anne M. Kelly-Rowley
23	2018	Wenyi Huang
24	2019	Amanda M. Palumbo
25	2020	Mark E. Jones
26	2021	Robbyn Prange
27	2022	Joel McDonald
28	2023	W. H. Hunter Woodward

2. Integrating Authentic Research Experience into Organic Chemistry Laboratory Course

David Baker

Delta College, University Center, 48710

Authentic research has been shown to cultivate a deeper appreciation for laboratory work and technical skills. It is an ideal opportunity for students to develop their own experimental problem solving and critical thinking skills. To provide this experience a research CURE (Course-based Undergraduate Research Experience) was embedded into the organic chemistry II laboratory course. The results of the student research work and future projects will be included. The student's experiences and views on these research activities, reporting and maintaining responsible and ethical conduct with research will be presented

3. An Evaluation of an Organic-Based Lab Experience in General Chemistry

Cassie Gardyszewski, Dr. Tomasik, Dr. Mueller, Dr. Marquez, Dr. Fahlman, Dr. Swartz

Central Michigan University, Mount Pleasant, 48858

For this project, a research-based lab contributing to the water purification research being conducted by Dr. Mueller, Dr. Marquez, and Dr. Fahlman, specifically focusing on the decarboxylation and the defluorination of perfluorooctanoic acid (PFOA), was implemented into an honors section of CHM 132. It was important to choose a staff-lead research project that introduces general chemistry students to concepts not typically introduced until typically the third or fourth year of a chemistry degree. This is important because it introduces key concepts that are essential to any researcher looking to pursue a degree in chemistry at an earlier time in their degree, allowing for a more solid understanding of what to expect in future classes.

For the students, the lab was split into two separate lab days, with the first being dedicated to preparing solutions and seeing how the reaction will be run, and the following lab period seeing how ¹⁹F NMR is performed and learning to analyze the resulting spectra. The students were surveyed on their experience with the lab, in terms of how they thought it impacted their learning, and how it prepared them for topics they will be learning further into a chemistry degree.

4. Synthesis and Characterization of Iron Single Atom Catalysts

Nathan Alchin

Central Michigan University, Mt. Pleasant, MI, 48859

Single atom catalysts (SACs) are isolated metal centers stabilized by neighboring surface atoms such as carbon and metal oxides. Compared to larger and bulkier catalysts, SACs have a better performance as they maximize the efficiency of catalytic centers while also maintaining stability. However, single atoms' high energy on a surface makes synthesis challenging. An effective method to meet this challenge is to use the strong interaction between the support atoms and the metal center. This research examines the synthesis of iron SACs using TEM and SEM imaging as well as x-ray diffraction.

5. Do Bees Dine with Their Neighbors? Analysis of Bee Pollen by Light Microscopy

Derek Schoch
Project Seed MSU St. Andrews

The objective of our research is to determine if bees in neighboring hives have similar preferences for where they gather pollen. Our group analyzed multiple samples of pollen collected simultaneously by bees in adjacent hives to determine if they are visiting the same or different flowers.

6. Analysis of Beer Antioxidants and the Aging of Beer

Brendan Pihaylic
Central Michigan University, Mt Pleasant, 48858

Oxidation during the post packaging (shelf-life) of fermented beverages has a significant impact on the quality of the product. Low volume production facilities (micro-breweries) desire to produce unique products. However, these designed variations and the inherent batch to batch variations continually change the product formulation, which inherently causes changes in the shelf-life of the product. Compounding these variations is distribution and the consumer may or may not refrigerate product prior to consumption. The goal of our project is to use HPLC to analyze the flavor stability and shelf-life for beer sent out for sale by evaluating its inherent antioxidant properties. Utilizing 2,2-diphenyl-1-picrylhydrazyl (DPPH) a stable free radical that can assess the antioxidant capacities of the beer components, in particular the alpha and beta humulones presented will be the HPLC developed technique. The research seeks to answer if correlating the antioxidant properties of the acid content to shelf life. And can this be used to predict product viability during the packaging stage of production?

7. Investigation Into the Link Between Fecal Contamination and Waterbody Qualities

Tristan Mosher
SVSU, University Center 48710

During the summer of 2023, The Saginaw Bay Environment Science Institute (SBESI, based in SVSU) continued an annual survey that has been conducted each year since 2012. As was the goal each prior year, fecal contamination levels were monitored during the summer beach season to ensure the safety of recreators in Bay County and Iosco County. In addition, an investigation into the correlation between fecal contamination levels and several variables was conducted. The variables in question included amount of rainfall prior to sample collection and the temperature, dissolved oxygen content, and turbidity of the water. Out of these, none were strongly correlated. Temperature appeared to have a moderate negative correlation to contamination levels, while dissolved oxygen content and amount of rainfall seemed to be uncorrelated or mildly correlated. Rainfall, however, has been found by SBESI to be at least moderately correlated to contamination levels due to runoff drainage into water bodies. It is possible rainfall data collected was not entirely accurate since access to it was difficult to obtain and gave information pertaining to only a small part of Bay County. Aside from the results of the secondary investigation, SBESI

provided a valuable service to the residents of Bay and Iosco Counties. As has been the case for several years, SVSU worked in conjunction with Michigan's Department of Environment, Great Lakes, and Energy to provide recreators with information on the safety of local water bodies, and shutting them down when deemed necessary.

8. Total syntheses of Aspidostomides D, E and F via unprecedented Strecker reaction on Indole

Konika Konika

Michigan State University, East Lansing, 48823

Pyrroloperazinone scaffold is one of the salient features of bromopyrrole alkaloids possessing various biological activities, including cytotoxic, antibiotic, antitumor, and growth inhibitory activities against various cell lines. Due to their potential applications as pharmaceuticals, synthesizing this scaffold has become an attractive research focus. Bromopyrrole alkaloids isolated from Patagonian Bryozoan *Aspidostoma giganteum* contain indole analogue of pyrroloperazinone scaffold. Aspidostomides D, E, and F contain indolopyrroloperazinone in their core structure. These natural products were evaluated against 786-O renal carcinoma cell line and Aspidostomide E was found to be moderately active. The natural scarcity of these alkaloids inhibits their further biological evaluation. This research work describes a novel and concise route to synthesize the scaffold which would facilitate their biological evaluation. α -amino nitriles are used as the starting materials, which can be easily synthesized via well-known Strecker synthesis from commercially available aldehydes. The final key cyclization is accessed via Bischler-Napieralski type reaction. Late-stage derivatization provides access to Aspidostomides D, E and F.

9. Synthesis of methyl gallate-based generation 2 antioxidant dendrons

Nanzhu Li

Central Michigan University, Department of Chemistry & Biochemistry, Mount Pleasant, 48859

Antioxidants neutralize harmful free radicals produced by metabolism, lifestyle, and many other environmental factors. Antioxidant dendrimers carrying multiple hindered phenolic groups on the surface are shown to have high antioxidant capabilities, particularly when stabilized by nearby electron-donating groups. Dendrimers, molecules with branching structures, are of particular significance due to their customizability and ability to have multiple functionalities. Dendron is a segment of a dendrimer and can be attached to another dendron to make a dendrimer. In this presentation, we will present the synthesis of a methyl gallate-based generation 2 dendron whose surface consists of syringaldehyde (hydrophobic).

10. Determination of the Efficacy of Biochar in Removing Antibiotics from Aqueous Solution

Warren Jacobs

Saginaw Valle State University, University Center 48710

With the rise in use of conventional antibiotics for the treatment of bacterial infections, the prevalence of antibiotic pollution in streams and waterways has become an issue of great importance. If left untreated, antibiotic pollution in water systems may help to accelerate the rate at which virulent bacteria develop natural resistance to antibiotics. In this project, the efficacy of biochar, an organic compound produced from the pyrolysis of biological matter, in the removal of tetracycline, sulfamethazine, 4-nitroanaline, and amoxicillin trihydrate all water-soluble antibiotics or antibiotic precursors commonly used for the treatment of infectious diseases will be determined. Furthermore, the efficacy of commercial and lab-synthesized biochar which have been magnetized with iron was compared to unmagnetized commercial and lab-generated biochar. In general, it was observed that commercial biochar samples were more effective at removing the target compounds from solution, with sulfamethazine showing the greatest difference in removal efficacy between the commercial and lab generated. When comparing magnetized and unmagnetized biochar, it appeared that magnetization of biochar did influence the capacity of biochar to remove antibiotics, though no consistent overall trend was observed when comparing different classes of antibiotics. Moving forward, further work will be performed in order to test biochar's absorptive capacity on other antibiotic compounds and determine the differences in affinity biochar has for differing antibiotics.

11. Synthesis, characterization, and electrochemical analysis of synthetic biomolecule models containing ruthenium with hydroxamate and/or nitrosyl ligands

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Previous studies have examined the interactions between biological models and nitric oxide (NO), though there is still research to be done on molecules capable of generating NO within biological systems, such as the heme unit. NO can be donated by hydroxamic acids, a molecule often used by the pharmaceutical industry. Thus, this research has worked to synthesize a model heme unit using d8-metal base, attaching a known NO-donating compound, hydroxamic acid, and studying their interactions. Using electrochemical and spectroelectrochemical techniques, the redox behavior of the compound interactions will be analyzed. It is hypothesized that the synthetic heme-hydroxamate model will be redox active. Spectroelectrochemistry will provide more data for the redox behavior, allowing an understanding of the ability of hydroxamate to donate NO. If these compounds bind a d8 metal, and are being used in pharmaceuticals, it is important to determine if they will also react with iron containing proteins and/or donate NO in a redox environment. This research therein provides insight to the potential side effects to pharmaceutical drugs containing NO-donors which may be currently unknown.

12. Actin Interactions with the Actin Crosslinking Domain of MARTX from *Vibrio cholerae*

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Cholera is a potentially fatal disease caused by the toxigenic bacteria known as *Vibrio cholerae*. These bacteria can target actin using a Multifunctional-Autoprocessing Repeats-in-Toxin (MARTX) with an actin crosslinking domain (ACD), causing actin to crosslink into oligomers. The important pieces of the ACD that interact with actin are unknown and requires further investigation. To do this, a construct was created through bacterial transformation, using plasmids with the ACD. Once purified, this plasmid was used as a template to make an expression construct for a polymerase chain reaction (PCR) and then verified through agarose gel electrophoresis, however these tests have not shown positive results for the expected construct. Variations of the PCR have been tested to troubleshoot these results, including using different primers and different volumes of template and nucleotides. These troubleshooting experiments are ongoing to verify that the purified plasmid is the expected construct to be used in future cloning experiments. Once this construct is confirmed, it will be used to build a fusion construct between the ACD and the biotin ligase BirA gene. The fusion protein will then be expressed and purified by the construct before being incubated with actin *in vitro*. This incubation will be analyzed using sodium dodecyl sulfate–polyacrylamide gel electrophoresis (SDS-PAGE), and western blot analysis to observe biotin attachment to actin. By obtaining these indirect measures of interaction between the ACD and actin, we will be able to further define how the ACD binds to its substrates.

13. RNAi Screen for RNA binding proteins that enhance microRNA activity after dauer diapause in *C. elegans*.

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Animal development occurs in the context of variable environmental conditions. Some animals can pause their development in a diapause stage to withstand adverse conditions. The effects of diapause on development are poorly understood. We address this question using the *C. elegans* model system. In favorable conditions, *C. elegans* larvae develop continuously through four larval stages. In adverse conditions, *C. elegans* larvae can enter a stress-induced and developmentally arrested stage called dauer. After dauer, *C. elegans* larvae display the same developmental outcomes as their continuous counterparts. One factor contributing to these outcomes appears to be the modulation of microRNA activity. MiRNAs and associated proteins bind to the 3'-UTR of target mRNAs to silence protein production. This gene silencing complex is named the miRNA-induced silencing complex (miRISC). *alg-1* and *alg-2* encode the core Argonaute proteins within the miRISC complex in *C. elegans*. These proteins function semi-redundantly. When *alg-1* is absent in continuously developing worms, various developmental phenotypes are observed. Most prominently, the vulva of the adult worm bursts or protrudes. However, when this same worm strain enters dauer and subsequently recovers, no bursting or protrusion occurs. We hypothesize that this phenotypic suppression is the result of increased miRNA activity post-dauer due to the action of RNA-binding proteins (RBPs). Our experiments aim to identify the RBPs that modulate miRISC. We have performed RNAi screens to identify genes that cause bursting or

vulval protrusion in post-dauer *alg-1*(null) adults. Thus far, we have screened 27 RPB-encoding genes and found that *rpb-8*, *lars-1*, *eef-1B.1*, *mcm-6*, and *aco-2* are all required for *alg-1*(null) animals to develop without vulval defects. This work is expected to provide insight into mechanisms by which microRNA pathways are modulated as well as the genes and their functions within the miRISC complex.

14. Developing and Optimizing Bioluminescent Neurotransmitter Sensors and Neuromodulators

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Many neurological diseases such as Alzheimer's Disease, Parkinson's Disease, and autism spectrum disorder have been shown to be caused, in part, by neurotransmitter dysfunction. Expanding on the types of neurotransmitters that can be detected is important to study the causes and treatments of these diseases. In this study, we focus on the amino acid gamma-aminobutyric acid (GABA), which is an inhibitory neurotransmitter found throughout the brain and is involved in many neurological disorders. We developed a variety of genetically encoded bioluminescent GABA sensors that are an attractive alternative to using fluorescent sensors because they do not require an excitation light source, allowing deeper areas of the brain to be recorded without damaging tissue and improving signal-to-noise ratio due to the lack of autofluorescence. We created a library of bioluminescent GABA sensor variants and tested them for improved responses to GABA. Taking bioluminescence readings on a plate reader, we found that the sensors with a mutated GABA binding domain and optimized linkers have higher responses to saturating amounts of GABA than the ones with the native GABA binding protein. To further improve the response of the sensors to GABA with the goal of using them to image brain activity in rodents, we will use rational design and further linker optimization to mutate amino acids in different areas of these GABA sensors with the goal of improving response amplitude and signal-to-noise ratio.

15. Progress toward developing a catalytically inactive hydrolase to selectively detect *Mycobacterium tuberculosis*

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Mycobacterium tuberculosis (Mtb), the causative agent of tuberculosis, infects nearly a quarter of the world's population and is responsible for the death of 1.6 million people annually. The mycobacterial cell envelope contains a unique, highly protective outer mycomembrane composed of long, hydrophobic mycolic acids. The mycolic acids are bound to trehalose 6-positions either as trehalose monomycolate (TMM) or trehalose dimycolate (TDM). TDM has previously been shown to be a virulence factor of Mtb. Since TDM is not a glycolipid that is naturally synthesized in humans or other microbes, it can serve as a biomarker for detecting Mtb. A novel strategy to detect carbohydrate-containing molecules with native structures using engineered, catalytically inactive carbohydrate-processing enzymes has recently emerged. Here, we utilize this strategy with a catalytically active and inactive TDM hydrolase (Tdmh) engineered to contain a poly-Histidine detection tag for their ability to detect TDM. Tdmh is a serine

esterase present in mycobacteria that hydrolyses TDM to TMM and a free mycolic acid. In its catalytically inactive mutant, Tdmh S124A, the catalytic triad serine (S) is substituted to alanine (A). We hypothesized that Tdmh S124A will maintain its binding specificity for TDM but lose catalytic activity. Detection of the mutant enzyme can be achieved using fluorescence or blotting. In this work, we expressed and purified the wild-type and mutant enzymes, confirmed catalytic activity, and evaluated the mutant enzyme's binding of TDM. If successful, this engineered enzyme has the potential to be a valuable new tool for detecting Mtb quickly and accurately.

16. Analyzing Perdew-Zunger Self-Interaction Corrections for Reaction Barrier Heights with Semi-Local Density Functionals: Unraveling the Evolution of Stretched Bond Errors

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The incorporation of self-interaction corrections (SIC) significantly improves chemical reaction barrier height predictions made using density functional theory methods. We present a detailed, orbital-by-orbital analysis of these corrections for three semi-local density functional approximations (DFAs) situated on the three lowest rungs of the Jacob's Ladder of approximations. The analysis is based on Fermi-Löwdin Orbital Self-Interaction Correction calculations performed at several steps along the approximate reaction pathway from the reactants (R) to the transition state (TS) to the products (P) for four representative reactions selected from the BH76 benchmark set. Across all three DFAs, our analysis reveals that the principal source of self-interaction error (SIE) in barrier height predictions is associated with the emergence of stretched bond orbitals near the transition state configuration. As an indicator of one-electron SIE, we introduce the X/C ratio, representing the ratio of self-exchange energy to self-Coulomb energy for a given orbital. While the exact, but unknown density functional has $X/C = 1.0$ for all orbitals, the practical DFAs under examination exhibit a range of X/C values. Significantly higher X/C values are observed in stretched or highly lobed orbitals. We demonstrate that significant differences in X/C values for corresponding orbitals in R, TS, and P configurations serve as a reliable indicator for identifying primary contributors to SIC in barrier heights and reaction energies. Our comparative analysis suggests that employing the SCAN meta-generalized gradient approximation, in conjunction with the Perdew-Zunger SIC approach, may have achieved the highest possible accuracy for semi-local functional predictions of barrier heights.

17. Antimicrobial properties of a diphenyl beta-lactone

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Antimicrobial resistance is a persistent health threat, killing an estimated 1.27 million people worldwide each year as microbes have developed defenses against compounds based on the cyclic amide beta-lactam functional group, which is commonly found in antibiotics as a cell wall synthesis inhibitor. However, in recent previous work, microbial susceptibility was seen in a novel compound based on beta-lactone ((3S,4E)-4-[1-(4-chlorophenyl)ethylidene]-3-methyloxetan-2-one), a cyclic carboxylic ester, against which no specific microbial enzymatic defenses are currently known.

Based on this observation, a simpler beta-lactone ((3R,4Z)-4-benzylidene-3-phenyloxetan-2-one) was synthesized via a facile one-pot reaction replacing a methyl group at the alpha carbon with a phenyl group to evaluate the effect of substitution on activity. The diphenyl beta-lactone was evaluated at varying doses (20 - 512 micrograms) against *E. coli*, *M. luteus*, *S. cerevisiae*, and *C. albicans*. All microbes demonstrated resistance across the doses studied in both disk diffusion and agar well trials, suggesting an essential structure-activity relationship at substituents located at the alpha carbon position.

18. Bioluminescent Kinase Sensors for detection of growth factor signaling in U87 glioblastoma cells.

Michael Chatterton
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Growth factor signaling is an important component of a large variety of cellular processes including metabolism, differentiation, proliferation, and migration. When growth factor signaling is altered it can lead to pathologies like cancer cells forming and proliferating within the body such as glioblastoma multiforme (GB). In this study, we focus on investigating and proposing novel therapeutic approaches utilizing genetically encoded Bioluminescent Kinase Sensors (BlinKS) to respond to growth factor signaling via kinases in the epidermal growth factor receptor (EGFR) signaling pathway. Specifically, this study is targeting the kinases within the MEK, RAS, RAF signaling pathway. To test our BlinkKS construct in association with U87 glioblastoma cells expressing our candidate sensor variants, treated the cells with epidermal growth factor (EGF) and measured the response of the BlinkKS sensors allowing for light emitted by the sensor and by measuring an optogenetic transcriptional readout via a fluorescent reporter protein. Bioluminescence readings were conducted on a plate reader, and it was found that the cells treated with EGF produced more luminescence than those treated with chlorambucil (a chemotherapy drug). Our sensors targeting this signaling cascade were also able to control an optogenetic transcription system, reporting EGFR activation with GFP expression. To further improve the BlinkKS sensor, we will be testing different substrate peptide variants as well as RAF mimic substrates to improve the sensors based on their effect. We ultimately aim to test these in rodents to reign in uncontrolled growth in cancer cells when using BlinkKS to drive expression of a therapeutic protein to halt cell division in response to EGF signaling.

19. Design and Synthesis of Mycolic Acid Probes to Investigate the Mycobacterial Outer Membrane

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Mycolic acids are unique long-chain fatty acids that are found in the cell envelope of Mycobacterium tuberculosis and other mycobacterial species, which include the pathogen that causes tuberculosis. Mycolic acids are responsible for M. tuberculosis survival within, and virulence against, the human host. The proteins that are involved in the biosynthesis and transport of mycolic acids could represent novel targets for tuberculosis diagnosis and drug development. Therefore, the synthetic mycolic acid probes that can provide insight into these processes would be beneficial. In this study, mycolic acid derivatives were synthesized with the unusual native functionalities intact, including the β -hydroxy group and α -alkyl branch. At the end of one lipid chain, a bioorthogonal tag (azido group) or fluorescent tag (fluorescein or BODIPY) were included as moieties to enable tracking and imaging of the probe in live cells. In addition to the synthetic studies, here we report on preliminary experiments testing the probes for uptake by wild-type Mycobacterium smegmatis.

20. Systemic Delivery of G4 PAMAM Dendrimers-Progesterone complex Intraperitoneally in MCAo Rat Models

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Stroke cause brain damage due to interrupted blood flow, resulting in disability and death. Prompt treatment and minimizing complications are crucial in managing stroke. Progesterone has neuroprotective and anti-inflammatory properties but delivering it across the blood-brain barrier (BBB) is challenging. This study investigated the effects of using G4 PAMAM dendrimers to deliver progesterone in a rat model of middle cerebral artery occlusion (MCAo). The rats were administered 10 intraperitoneal injections of 8mg/kg of progesterone-dendrimer, dendrimer only, or HBSS solution every other day, starting 1 week after surgery, with the last 2 doses reduced to half to prevent withdrawal. Functional motor tests were conducted weekly, including the ladder test, cylinder test, and Garcia Neurological Scoring. Preliminary analysis of the ladder test showed motor coordination improvements in stroke rats treated with dendrimer and progesterone dendrimer. The cylinder test also showed improvement in motor function in the dendrimer-treated stroke rats. Initial results from the neurological scoring data in stroke rats treated with progesterone-dendrimer showed motor improvement and a reduced time to recover from the infarct. The study demonstrates that dendrimers can cross BBB and the dendrimer delivery system is an effective mechanism for delivering progesterone treatment intraperitoneally in middle cerebral artery occluded rat models. Preliminary results suggest that this delivery system could

decrease motor deficits and improve outcomes in stroke patients. Further studies are needed to confirm these findings and establish the optimal dosing and treatment duration.

Support for this study was provided by the American Heart Association (957277), Neuroscience Program, College of Medicine, Department of Chemistry and Biochemistry, John G. Kulhavi Professorship in Neuroscience, and E. Malcolm Field and Gary Leo Dunbar endowed Chair in Neuroscience at Central Michigan University and partially by the Summer Scholar program received by King, M. at Central Michigan University College of Medicine.

21. Synthesis and characterization of trehalose-biotin conjugates as tools for the detection of mycobacteria

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In 2021, approximately 1.6 million people died of tuberculosis, and it is the second leading infectious killer only preceded by COVID-19 according to the World Health Organization. The detection of the causative agent *Mycobacterium Tuberculosis* (Mtb) is a slow and complicated process, making it difficult to diagnose tuberculosis, including drug resistant forms. Trehalose is found in Mtb in the form of the glycolipids trehalose monomycolate (TMM) and trehalose dimycolate (TDM) which are in the outer membrane of the mycobacteria. Free trehalose is also present in the cell, as it is synthesized in the cytoplasm and also released during the synthesis of TMM and TDM through antigen 85 (Ag85) and is recycled into the cell through the transporter LpqY-SugABC. Using trehalose probes, the trehalose metabolic pathway may be hijacked so that the labelled trehalose may enter the cell and incorporate into mycomembrane glycolipids. For example, azide- and fluorophore-modified trehalose analogues are able to incorporate into the cell membrane to allow for visualization of the cell surface glycolipids. In this project, trehalose-biotin conjugates with variable length PEG linkers were synthesized to enable testing of the compounds as potential Mtb detection tools. The biotin molecule incorporated into the bacterial surface is hypothesized to facilitate the rapid and selective enrichment and/or detection of Mtb from complex samples by using biotin-binding avidin reagents.

22. Screening Trehalose Synthase Variants for Substrate Tolerance with Trehalose Analogs for the Inhibition of Mycobacterium tuberculosis.

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One factor that causes virulence in *Mycobacterium tuberculosis*, the bacterium that causes tuberculosis (TB), is the metabolism of trehalose. However, we can also target trehalose metabolism as a method to stop TB virulence. One interesting candidate for inhibition of trehalose metabolism is the trehalose analogue 2-trehaloseamine, because it is a potent mycobacterial growth inhibitor. However, challenges with synthesizing it makes access to this analogue limiting. One project in our lab is the chemoenzymatic synthesis of trehalose analogs using trehalose synthase (TreT) from *Thermoproteus tenax*. One challenge of this process is the limited substrate tolerance, that gives rise to 2-trehaloseamine. In this project we screened trehalose synthase enzymes from other sources to test for better substrate suitability. To do this, UDP-GloTM, a luminescence-based glycosyltransferase assay was utilized. This assay is used to detect the activity of glycosyltransferase enzymes, which includes trehalose synthase. The activity is measured by the amount of free UDP generated in the reaction between a glucose analog and UDP-glucose. This assay was performed in triplicate with the following enzymes mCherry-TuTreT, mCherry-TtTreT, mCherry-TnTreT, and TreT. All four enzymes were tested with nine different substrates, most notable being 2-azido glucose, the compound used to make trehalosamine. From one trial it was found mCherry-TuTreT showed activity with 2-azido glucose, whereas the others showed no activity with it. However, because this finding was only after one trial, more trials must be performed before we can confidently say mCherry-TuTreT has substrate suitability with 2-azido glucose. In conclusion, while mCherry-TuTreT shows potential substrate suitability with 2-azido glucose, more trials must be performed. If confirmed, this could offer a more efficient way for obtaining a promising inhibitor of *Mycobacterium tuberculosis*.

23. Enhancing Biochemical Insights Within the Brain via Q-ball Imaging

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The intricate neural architectures within the brain, including crossing, kissing, and twisting fibers, are closely tied to the underlying biochemistry of neural function, signaling, and health. To enhance our knowledge of brain structure, we study Q-ball imaging, a magnetic resonance imaging (MRI) technique. We utilize signal data measured on a spherical domain to create an Orientation Distribution Function (ODF). This ODF encapsulates angular information, revealing the likelihood of diffusion displacement for water molecules. Yet, obtaining signal data from many diffusion gradient (DG) directions often results in extended scan times. To overcome this issue, we suggest capturing signals at a relatively limited set of DG directions and estimating the signals for additional DG directions by employing k-nearest neighbors (k-NN) regression. When comparing the k-NN regression approach to two other existing methods, our findings consistently demonstrate its superiority in improving signal estimation, ODF estimation, and major direction detection accuracy and reliability.

24. Host-directed immune targeting of mycobacteria through cell surface glycan engineering

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Non-tuberculous mycobacteria (NTM) pose a growing threat as a cause of severe pulmonary disease, particularly in immunocompromised individuals. Conventional antibiotic treatments often fall short due to the intrinsic drug tolerance conferred by the unique mycobacterial cell envelope, leading to acquired drug resistance. To address this challenge and explore novel therapeutic approaches, we developed a strategy to selectively modify the mycobacterial cell surface glycans with antibody-recruiting molecules (ARMs). These ARMs serve as molecular tags, facilitating the binding of human-endogenous antibodies to the bacteria and enhancing macrophage effector functions. Our previous work synthesized a mycobacteria-specific ARM composed of a trehalose-targeting moiety and a dinitrophenyl hapten (Tre-DNP). This ARM demonstrated specific incorporation into the surface glycolipids of *Mycobacterium smegmatis* through trehalose metabolism. By recruiting anti-DNP antibodies and promoting phagocytosis, we successfully validated the proof-of-concept for this approach. Building upon these findings, we have expanded our investigations to include *Mycobacterium abscessus* and *Mycobacterium avium*. We have demonstrated that the ARM can effectively label these NTM species and enhance uptake by macrophages, further validating its potential as a therapeutic tool. This feature underscores the versatility of the reported ARM and its potential to be harnessed in developing immune-targeting strategies against NTM and diverse mycobacterial pathogens.

25. Synthesis of carnosine-based aqueous-soluble antioxidant dendrimers for biomedical applications

Blessed Agbemade

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Oxidative stress produced by free radicals during metabolism, stress, infection, inflammations, and exposure to environmental factors may lead to health repercussions such as diabetes, cancer, cardiovascular and neurodegenerative diseases. Polyphenols are well known for scavenging free radicals and providing various health-related benefits. However, most of the phenolic antioxidants are not aqueous-soluble, decreasing their bioavailability. In this presentation, we will report synthesis of two water-soluble dendritic antioxidants, which were synthesized using L-carnosine as the core and vanillin and syringaldehyde as building blocks. We will also present their DPPH radical scavenging activities, DNA protective effects against free radicals, and their pro-oxidant potentials.

26. Targeting Mycobacterium tuberculosis persistence through inhibition of the trehalose catalytic shift

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Trehalose, a non-mammalian disaccharide consisting of two glucose molecules joined by a 1,1- α , α -glycosidic bond, is a major component of cell wall-associated glycolipids in *Mycobacterium tuberculosis* (Mtb). Trehalose also plays a significant role in biogenesis and remodeling of the mycobacterial outer membrane. The metabolic pathways associated with trehalose-mediated mycolic acid transfer are conserved in mycobacteria and essential for viability, and thus represent promising targets for drug development. In a collaborative study, we discovered that 6-azido-6-deoxy-D-trehalose (6-TreAz) (i) selectively inhibits Mtb biofilm formation by disruption of TreS-mediated trehalose metabolic remodeling; and (ii) sensitizes drug-tolerant Mtb to the existing anti-TB compound bedaquiline. Thus, 6-TreAz and related trehalose analogues, can potentially serve as valuable tools for understanding mycobacterial trehalose metabolic remodeling and exploiting it to develop novel adjunctive therapeutics for TB. Here, we report the synthesis of a panel of azido and amino-trehalose analogues and evaluation of these compounds as inhibitors of Mtb growth and biofilm formation. Given the challenges of chemical synthesis of trehalose analogues, we enlisted the glycosyltransferase enzyme TreT to chemoenzymatically synthesize most of the target compounds. From the compound panel, multiple analogues were shown to selectively inhibit Mtb biofilm formation with better potency than 6-TreAz, and the mechanism of action was investigated using knock-out mutants and metabolomics. These compounds can serve as tools to investigate mycobacterial trehalose metabolism and potentially serve as lead compounds in antibiotic development.

27. An in-silico pipeline for the rational directed evolution of light-sensitive transcription factor EL222

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Directed evolution is a technique for improving protein activity and stability for use in translational and basic research. Two approaches exist: random and rational evolution. With random evolution, libraries of hundreds of thousands of variants are produced with procedures like DNA shuffling and error-prone PCR. On the other hand, rational mutagenesis takes advantage of thoroughly assessed and understood amino acid sequences and/or three-dimensional structures of target proteins to generate variants without large structural and functional disruptions, while decreasing library size^{2,3}. To minimize library size and improve ease of medium throughput screening in mammalian cells, I developed an in-silico pipeline for rational mutagenesis dependent on multiple sequence alignment (MSA) of homologous proteins, identification of functionally significant residues, and back-to-consensus mutagenesis. I applied this pipeline to the light-sensitive transcription factor EL222 to produce variants capable of facilitating higher levels of transcription when stimulated with light. Homologous proteins were aligned using the program MUSCLE to form a consensus sequence. The MSA was then fed into the program ConSurf to identify

functionally significant residues in EL222 using Max Likelihood statistics and conservation of residues at each position. To generate the library, residues that were functionally significant and differed from the consensus sequence were mutated to match the consensus at the same location. By making one amino acid conversion per variant, I was able to develop a library of 93 mutants. Four different variants were identified with higher levels of transcription than wildtype EL222, the best of which is the mutation D61A.

- [1] Goldsmith, M. & Tawfik, D. S. Enzyme engineering by targeted libraries. *Methods Enzymol*, 523, 257-83 (2013).
[2] Jochens, H. & Bornscheuer, U. T. Natural diversity to guide focused directed evolution. *ChemBiochem*, 11, 1861-6 (2010).
[3] Sebestova, E., Bendl, J., Brezovsky, J. & Damborsky, J. Computational tools for designing smart libraries. *Methods Mol Biol*, 1179, 291-314 (2014).

28. Development of degradation-resistant trehalose analogues: leads for treatment of cardiometabolic disease and inhibition of microbial pathogens

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Transdermal administration of a non-steroidal anti-inflammatory drug (NSAID) is highly recommended over oral intake for chronic conditions like arthritis pain. Delivering the right amount of drug in a sustainable fashion for an extended time using a more patient-compliant dosage form is strongly desired. Being a primary constituent in the modern matrix-type transdermal skin patch formulations, the pressure sensitive adhesive (PSA) technologies play a key role not only in the patch adhesion to the skin but also in the delivery of drug. PSA technologies typically used include polyisobutene, acrylic and silicone. While individual PSA may fulfil the needs sporadically in patch formulations, the advantage of using a blend of PSA technologies has been demonstrated in this study to deliver a model drug diclofenac base (DCF) efficiently. With other variables kept constant including [DCF] at 2%, a patch formulation made using acrylic PSA delivered about 54 μ g, a patch formulation made using silicone PSA delivered about 96 μ g, whereas a patch made using a blend of acrylic and silicone PSA delivered about 122 μ g. The result was obtained when patches were tested in-vitro for DCF permeability through human cadaver epidermis for 48 hr at 32°C. The right ratio of PSA blends in the patch formulations also showed the possibility of attaining higher DCF delivery rate than that by patch formulation containing acrylic PSA or acrylic-rich PSA blends. The patch formulations containing PSA blend was also found performing best in terms of patch adhesion and DCF's solubility in the patch.

29. Pectin-Stabilized Gold Nanoparticles: An Insight Mechanism of Targeted Drug Delivery

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The use of nanoparticles as a drug delivery system has become one of the most promising strategies. Thus, we have developed recent advances in targeted drug delivery using natural polysaccharide (Pectin) for synthesis of colloidal gold nanoparticles (Au-NPs).

Asialoglycoprotein (ASGP) receptor is mainly expressed on the surface of liver cells, which can be recognized specifically by the galactose residues of ASGP. As a proof of concept, the targeting efficacy can be improved significantly via receptor mediated endocytosis. Considering the large number of binding sites in hepatocytes for ASGP and the high affinity between them, modification of drug delivery systems with galactose residues represents an efficient approach toward liver and targeted drug delivery.

Pectin is predominantly a linear polymer mainly composed of poly-D-galacturonic acid residues and used as stabilizing and capping agent for green synthesis of Au-NPs. Various formulation and process parameters such as temperature, time, and concentration were optimized for synthesis of Au-NPs and further evaluated using dynamic light scattering systems, powder x-ray diffraction, high-resolution transmission electron microscopy and atomic force microscopy.

In addition, the pectin-based gold nanoparticles exhibit prolonged in-vitro drug release as well as better stability profile in physiological conditions (pH). Taken together, the targeting efficiency of proposed system was evaluated in preclinical (living animal) studies using non-invasive in-vivo imaging system. Therefore, the developed formulation strategy of pectin-stabilized gold nanoparticles could be utilized as a promising platform for the targeting and treatment of various liver disorders.

Keywords: targeted drug delivery; pectin; gold nanoparticles; preclinical studies.

30. NIR-assisted stereolithography for high performance polymer derived ceramic

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The utilization of stereolithography (SLA) in the production of 3D structured ceramic materials derived from polymers (known as PDC materials) has significantly enhanced precision, production efficiency, and the ability to craft intricate ceramic shapes. However, when working with PDC composites, traditional UV-assisted SLA encounters notable challenges, including limited light penetration, restricted particle loadings, substantial shrinkage, and subpar mechanical properties of UV-polymerized and pyrolyzed components. In this study, a new NIR-assisted thermal SLA printing technique is introduced to address these issues. This innovative thermal method employs a high-intensity NIR laser to induce localized thermal effects, resulting in the rapid solidification of the resin during scanning through a thermal curing process. The technology was demonstrated using a gantry-based setup and a resin pool in a top-down SLA configuration. This approach facilitated the creation of ceramic matrix composite materials primarily composed of SiC, SiOC, and SiCN, reinforced through this thermal curing approach. Furthermore, the use of thermal curing chemistry, as opposed to UV curing, broadens the horizons for printing novel polymers,

enabling additional mechanisms such as hydrosilylation, epoxides ring opening, and esterification within the thermal printing process.

31. Removal of Arsenate and Ammonia from Water by Adsorptive Membranes and Resins

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The presence of arsenic and ammonia in ground and surface waters has resulted in severe adverse effects to human health and the environment. Adsorptive resins and membranes have been used for the removal of these contaminants. However, selectivity and permeability of these materials still needs to be improved. In this work, adsorbents and adsorptive membranes were prepared using molecularly imprinted acrylate polymers templated for arsenate and ammonia and reinforced with graphitic carbon nitride. The developed adsorbent removed arsenate at a capacity and selectivity similar to commercial ion-exchange resins. Ammonia was removed at higher capacity than commercial ion exchange resins but showed lower selectivity. Non-imprinted controls were used for analytic comparison, and in experimentation demonstrated less removal than the prepared membranes. While the prepared membranes performed as well or better than competition commercial resins, further optimization is required to improve stability and selectivity.

32. Facile Route for Polyether Bioconjugation via a Functional Hydroxysuccinimidyl Ester Initiator

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Poly(ethylene glycol) (PEG) is the most widely used polymer in pharmaceutical applications due to its biocompatibility, ability to enhance drug solubility, controlled release, prolonged circulation time, and reduced immunogenicity. The coupling of PEG to a therapeutic moiety often requires post-modification of the chain termini in order to introduce functional groups selective to the available reactive groups on the target moiety, one of the most common being succinimidyl esters that readily react with lysine residues on proteins. To mimic traditional bioconjugation/PEGylation strategies, an NHS dimethyl aluminum initiator (NHS-SAl) was synthesized and used to directly incorporate an NHS terminus with a function initiator (α -functionalization) in multifunctional PEG derivatives, poly(propylene oxide), poly(epichlorohydrin), and poly(allyl glycidyl ether). NHS-SAl can be easily synthesized from the reaction of an N-hydroxy succinimide ester and trimethylaluminum. The structure and kinetics of polymerizations initiated from NHS-SAl were investigated to gain an understanding of the synthetic methodology, as well as structural and composition capabilities. Polymer end group reactivity was confirmed by coupling to amine-modified silica nanoparticles, poly(ethyleneimine), and other small amine-containing molecules. Overall, a novel synthetic route for multifunctional PEG derivatives with direct incorporation of a terminal NHS group by α -functionalization was established, potentially simplifying polymer conjugation methods.

33. Evaluation of Stress-Strain and Fracture Behavior in Patterned Hydrogels

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Hydrogels are elastic and hydrophilic soft matter materials that have important uses in a variety of biomedical and robotic applications. The implementation of 3D patterned structures in hydrogel systems allows for the engineering of materials that more closely mimic the biological microenvironment, and patterned hydrogels have been fabricated to elicit smart deformation properties in response to stimuli. However, further investigation is needed on the tensile stress-strain behavior and fracture mechanics of this patterned structure. Degree of cross-linking is an important determiner of the mechanical properties of a hydrogel, but it is also important to consider how changing the hole and strut sizes in patterned samples may affect the final stress, strain, and method of fracture of the hydrogel. This work aims to investigate how the implementation of simple honeycomb patterned structures in poly(ethylene glycol) hydrogel systems affects the way the material responds to externally applied forces.

34. PEGylated Poly(amidoamine) Dendrimers Toward Translational Nanotherapeutics

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Dendrimers have made great progress since their discovery at the Dow Chemical Company (Midland, Michigan, USA) in the 1980s [1, 2]. These polyvalent nanostructures have emerged as promising candidates for many nanomedicine applications.

PEGylated dendrimers covalently coupled with a targeting ligand facilitate the delivery of therapeutics in targeted (active) and controlled manner. Small molecules such as hyaluronic acid (HA), a naturally occurring polysaccharide found to have high affinity for CD44 receptors, over-expressed on blood brain barrier (BBB) including, several tumors cell surfaces and glioblastoma (GBM). GBM is a malignant grade IV tumor, generally found in the cerebral hemispheres of the brain. World Health Organization, reports that the overall median survival of patient with GBM is approximately 11-15 months [3].

The chemotherapeutic drug (Docetaxel) used in the treatment of GBM suffers from poor BBB penetration, severe systemic toxicities, and lack of specificity towards tumor cells [4]. Thus, we report the synthesis and evaluation of PEGylated dendrimer HA-conjugate as nanosystems for site-specific delivery of nanotherapeutics. The resulting dendrimer nanosystems was evaluated by Nuclear magnetic resonance spectroscopy, Photon correlation spectroscopy, Fourier-transform infrared spectroscopy and UV-visible spectroscopy.

Storage stability of the PEGylated dendrimer HA-conjugate was determined and found to be stable over the period of 90 days. In addition, the proposed system showed improved targeting efficiency in preclinical (living animal) studies using non-invasive imaging system. Thus, our proposed system demonstrated high biocompatibility and excellent in-vitro, in-vivo and ex-vivo profiles which has shown great promise as a unique therapeutic application in various tumor related disorders.

References:

- [1] Tomalia, D.A., Baker, H., Dewald, J., Hall, M., Kallos, G., Martin, S., Roeck, J., Ryder, J. and Smith, P. A new class of polymers: starburst-dendritic macromolecules. *Polymer journal* 1985. 17(1), 117-132.
- [2] Tomalia, D.A., and Jean M. J. Fréchet. Discovery of dendrimers and dendritic polymers: A brief historical perspective. *J Polym Sci Part A: Polym Chem* 2002. 40: 2719–2728.
- [3] The 2016 World Health Organization Classification of Central Nervous System Tumors: An Era of Molecular Biology.
- [4] Current Challenges and Opportunities in Treating Glioblastoma. *Pharmacological Reviews* 2018, 70:412–445.

35. Impact of Templating Agent on the Photocatalytic Activity of Iron-Doped Graphitic Carbon Nitride

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Metal-doped graphitic carbon nitrides demonstrate promising photocatalytic activity in a number of reactions. Most currently available water treatments focus solely on adsorption, leading to significant challenges and costs associated with disposal. These costs could be averted through in-situ destruction of target contaminants. Iron-doped graphitic carbon nitride has significant potential in water treatment since it can both adsorb organic contaminants and subsequently destroy them through photocatalytic oxidation.

The catalytic capacity of Fe-g-CN has been shown to correlate with iron content through exfoliation of the graphitic sheets which are separated by the included iron. This spatial separation allows molecular targets of oxidation to access catalytic sites on the Fe-g-CN more readily. During synthesis, a templating agent (ammonium chloride) is included to aid in the separation of Fe-g-CN nanosheets. It is hypothesized that increasing the quantity of templating agent will further exfoliate the nanosheets, allowing more access to catalytic sites and improving the catalytic capacity of the product. To test this, Fe-g-CN produced using varying levels of ammonium chloride is used to catalyze the oxidative photodegradation of methylene blue dye.

36. Characterization of network heterogeneity in polymerized dental adhesives

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Heterogeneity and phase separation during network polymerization is cited as a major contributing factor to the poor mechanical durability and failure of dental adhesive materials. This study investigates how the ratio of hydrophobic crosslinkers to hydrophilic comonomer (C/H ratio), as well as cosolvent fraction (ethanol/water) influences the degree of heterogeneity and proclivity for phase separation in a simplified self-etch adhesive formulation.

Twelve model self-etch adhesive formulations were investigated, with 4 different C/H ratios (7:1, 2.2:1, 1:1, 0.5:1) and 3 different cosolvent fractions (0, 10 and 20 wt%). The heterogeneity and phase behavior of these formulations were probed using Fourier Transform Infrared Spectroscopy (FT-IR), dynamic mechanical analysis (DMA), small-angle x-ray scattering (SAXS) and atomic force microscopy (AFM) were employed for post-polymerization network analysis.

In resins without cosolvent, DMA, SAXS and AFM characterizations confirm a lower degree of nanoscale heterogeneity as C/H ratio decreases. However, when 10 wt% or 20 wt% of cosolvent is included in the adhesive formulations, a higher degree of heterogeneity and even distinct phase separation with domains ranging from a few hundreds of nanometers to a few micrometers in size form. This is particularly noticeable at lower C/H ratios, which is surprising as HEMA is commonly considered a compatibilizer between hydrophobic crosslinkers and aqueous solvents.

This work further investigated the driving forces of heterogeneity and phase separation during photopolymerization of model adhesive formulations. Our experiments demonstrate that formulations with lower C/H ratio and thus a lower viscosity experience later onsets of diffusion limitations during polymerization, which favors thermodynamically-driven phase separation. Therefore, to determine or predict the resulting phase structure of network dental materials, it is necessary to consider the kinetics and diffusion constraints during the formation of the polymer network.

37. Substrate-Free Polymer-Ceramic Nanocomposites for Energy Applications

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Flexible capacitors have emerged as top candidates for the design of portable, compact and wearable electronic devices for both military and domestic applications. Among the existing materials incorporated into flexible capacitors, polymer-ceramic nanocomposite films are preferred the most as they combine the innate excellent mechanical properties of the polymers with the high dielectric constant of conventional ceramics. We report here on the rational design of polymer-ceramic nanocomposite films obtained by dispersing ferroelectric BaTiO₃ filler nanoparticles (BaTiO₃, into two types of elastomers, namely an organic elastomer (Vistamaxx) and an inorganic one (polydimethylsiloxane (PDMS). Incorporation of 15 nm BaTiO₃ colloidal nanocrystals into each polymer host matrix by highly versatile, yet low-cost solution-based techniques developed by our group allowed us to design highly uniform

substrate free polymer-ceramic nanocomposite films with controlled thicknesses, composition and function-driven electrical and mechanical properties. The performance characteristics of each of these types of nanocomposite films were assessed by using various instrumental techniques, including spectroscopy, X-Ray diffraction, thermal analysis, electron and scanning probe microscopy and dielectric spectroscopy. Room temperature dielectric spectroscopy data showed that the dielectric constant of the SBS elastomer improved significantly whereas the breakdown field values were found to decrease upon incorporating the BaTiO₃ nanocubes and increasing their concentration within the polymer host matrix. The experimental results show that the nanocomposite films fabricated by the proposed approach present high permittivity values along with excellent mechanical properties which can be potentially used in energy storage applications.

38. Chemically and Physically Patterned Polymer Surfaces of Photopolymerization Induced Phase Separating Resins Using Interfacial Interactions to Guide Surface Morphology

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Hierarchical, topographical surface structures are abundant in nature, from beetle carapace to plant leaves. Multi-level patterning enhances these surfaces, resulting in unique wettability, adhesion, and self-cleaning behavior. Photopolymerization induced phase separation (PIPS) can mimic these heterogeneous materials by using initially miscible resin solutions that phase separate during curing. PIPS holds promise for complex surfaces as leverages two methods for generating surface wrinkling: a depth-wise modulus gradient facilitated by oxygen quenching of radicals as well as depth-independent modulus gradients from phase separated domains that form within the 3D bulk of the sample. Additionally, introducing multiple interface types for the resin to be in contact with during photopolymerization allows for further manipulation of spatially-distinct domains. In this work, we investigate in-situ phase separation and surface roughening using resins consisting of vinyl acetate and 1,6-hexanediol diacrylate monomers with poly(dimethyl siloxane) inert polymer additives. As opposed to traditional lithography which creates regions of cured and uncured material, our technique patterns regions of differing surface energies in a single procedure, verified through contact angles and surface profilometry. We demonstrate how considering the thermodynamic compatibility between chemical species and the impact of reaction kinetics during phase separation can lead to multi-scale textured surfaces with dissimilar chemical domains on the same surface. We demonstrate how this texturing and patterning can be manipulated via resin thickness, composition, and varying the time of liquid interface application. This approach is unique as we generate stark surface character contrasts and significant topography in a single step using initially miscible resins.

39. Investigating Instability Behaviors to Understand the Relaxation Dynamics of PEG Hydrogels

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Polymer gels are utilized in diverse applications ranging from ion-exchange membranes to drug delivery systems due to their ability to withstand the mechanical deformation associated with swelling and deswelling repeatedly. The three-dimensional, cross-linked hydrogel network enables such behavior by deforming in response to the internal stresses induced by swelling. When designing long-lasting, switchable properties, understanding the mechanisms that elastic polymer networks utilize to both generate and dissipate internal stresses during processes such as swelling is critical. However, limited research has been performed to understand the unsteady-state swelling regime of hydrogels prior to an equilibrium state where no more solvent diffusion occurs. This unsteady-state regime is important, as instabilities such as spontaneous rupture and surface buckling are observed during this period. Here we show that these instability behaviors are directly related to the dynamics of relaxation during swelling. By manipulating both the internal network constraints (e.g., cross-link density) and external diffusive pressure (e.g., solvent quality) present during swelling of poly(ethylene glycol) hydrogels, our work establishes a connection between observed instabilities and the mechanisms by which internal stresses are dissipated. Mainly, networks that undergo quick rearrangements dissipate stress through wrinkling, while those whose networks exhibit critical levels of constraint during swelling relieve stress through bulk fracture. These results serve as a fundamental understanding of how soft materials can respond to stresses through complex, dynamic deformation. With this knowledge, future design of hydrogel systems can be improved by utilizing the connection between polymer network relaxation and swelling mechanics. Engineering dynamic surface properties, while also mitigating unwanted instability, opens the door for emerging technology such as smart anti-fouling and sensors.

40. Synthesis of Organic Compounds for Sustainable Energy

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Organic redox flow batteries (ORFBs) are regarded as a viable alternative to the traditional lithium-ion batteries. ORFBs contain non-metallic, carbon based, organic molecules. Redox flow batteries are seen as one of the most practical alternatives for medium and large-scale energy storage applications. Large scale energy storage is necessary for the transition to more renewable yet intermittent forms of energy such as wind or solar power. Jolt Energy's goal is to innovate renewable energy storage. Redox flow batteries are constructed with external tanks containing electrolytes. The storage tanks are separate from the electrochemical cell, and the power and storage capabilities can be modified by changing the volume of the tanks. The ORFB we have produced uses the same organic molecule for both the anolyte and the catholyte, with the only difference being the oxidation states. ORFBs are inherently much safer than traditional lithium-ion batteries due to the separation of the anolyte and catholyte and the lack of volatility of the components, which is a fundamental consideration for large scale energy purposes. They are suitable for large capacity, long lifetime, low cost, and high safety. We propose using Structure-Activity

Relationships by chemically modifying the R groups to devise more effective structures. The R groups are the sites where different functional groups are used to maximize solubility, increase energy density, and increase reversible redox cycles, all while being environmentally acceptable.

41. Synthesis of graphitic carbon nitride functionalized with imprinted polymers for the removal of arsenate and ammonia in water

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Project SEED

The presence of arsenic and ammonia in ground and surface waters has led to significant adverse impacts on both human health and the environment. Various techniques, such as adsorption and membrane processes, have been employed to tackle these contaminants. However, the quest for materials with heightened capacity and selectivity remains ongoing. In this study, we crafted adsorbents and adsorptive membranes utilizing nanostructured graphitic carbon nitride adorned with molecularly imprinted acrylate polymers tailored for arsenate and ammonia. The resulting adsorbent effectively eliminated arsenate, mirroring the capacity and selectivity of commercial ion-exchange resins. When it came to ammonia removal, our adsorbent outperformed commercial ion exchange resins in terms of capacity, albeit with slightly reduced selectivity. Furthermore, our specially prepared membranes exhibited superior arsenate and ammonia removal capabilities compared to non-imprinted counterparts, even when competing with abundant ions in the water. Nevertheless, further enhancements are necessary to improve pressure stability, capacity, and selectivity.

42. Dental Adhesives

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This research involves the analysis of two samples of dental adhesives. The first sample is a self-etch adhesive, while the second sample is a self-etch adhesive paired with a desensitizer. Self-etch quality, however, allows for priming without rinsing due to the acidic nature of the content. Desensitizers are known to relieve tooth sensitivity after restorative preparations but are not critical to a solid preparation and are usually used at the discretion of the doctor. These dental adhesives are complex mixtures. They were analyzed by IR, NMR, and Mass Spectrometry and the details will be presented.

43. Utilization of Additive Manufacturing for Biopolymer (PCL and PLA) Scaffolds in Facilitating Trabecular Bone Osteogenesis

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The natural healing of trabecular bone through osteogenesis takes several months and many common tissue engineering methods have associated problems such as risk of infection and rejection. The usage of alloplastic scaffolds is an alternative treatment that can effectively bypass these problems. By utilizing additive manufacturing (AM), the scaffolds were optimized mechanically and biologically and could be customized to the injury site in the future. The infill structures under study were Triply Periodic Minimal Surfaces (TPMS), known for their high surface areas and resemblance to trabecular bone morphology. TPMS-infill scaffolds (6 mm H x 5 mm D cylinder) designed to fit into 96-well cell culture plates were seeded and incubated with *E. coli* in order to simulate mesenchymal stem cell attachment. Three TPMS (Gyroid, Diamond, Schwarz-P) structures and one control non-TPMS (NT) structure, fabricated with non-toxic and biodegradable polymers (polylactic acid and polycaprolactone), were tested and the bacterial growth was isolated and plated. The resulting colony-forming unit (CFU) assays suggest that the greatest growth occurs on high-surface-area TPMS structures in comparison to the NT structure. The results will provide guidance for future experiments regarding osteoblast differentiation using three-dimensional scaffolds at the University of Michigan Flint Biology Lab.