JAMES MADISON UNIVERSITY®

DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

49TH ANNUAL SPRING UNDERGRADUATE RESEARCH SYMPOSIUM

THURSDAY APRIL 24, 2025

ORAL SESSION I: 11:00AM – 12:00PM (KING 259)
ORAL SESSION II: 1:00 – 2:30 PM (KING 259)

FRIDAY APRIL 25, 2025

POSTER SESSION: 1:00 – 3:00 PM (PCB LOBBY)
SPECIAL ANNOUNCEMENTS: 3:30PM (KING 159)
KEYNOTE ADDRESS: 3:35 – 4:35 PM (KING 159)

49th Annual Department of Chemistry and Biochemistry
Spring Undergraduate Research Symposium

Keynote Speaker

Paris Hamilton, PhD
(JMU Class of 2009)
Associate Director of Regulatory Affairs
Chemistry, Manufacturing, and Controls (CMC)
Agios Pharmaceuticals
Cambridge, MA

Paris Hamilton is an Associate Director of Regulatory Affairs Chemistry, Manufacturing, and Controls (CMC) at Agios Pharmaceuticals, where he supports the development of therapeutics for a variety of rare diseases. He earned his Bachelor of Science in Chemistry from James Madison University in 2009, where he conducted undergraduate research on the self-assembly of propargylic alcohols under the guidance of Dr. Kevin Caran.

Paris went on to earn both his M.S. and Ph.D. in Chemistry from Clemson University. His graduate work focused first on the biophysics of DNA/RNA drug binding (M.S.) and later on the site-specific short-chain PEGylation of peptide analogues (Ph.D.). During graduate school, he completed a year-long medicinal chemistry internship at GlaxoSmithKline, where he synthesized complex small molecules through multistep pathways.

Following his studies, Paris joined a mid-sized pharmaceutical company, where he supported R&D efforts across formulation development, analytical method validation, manufacturing scale-up, stability studies, and regulatory submissions. He later held roles as a supervisory chemist at the NIH Clinical Center, a review chemist at the FDA, and a pharmaceutical consultant prior to his current position at Agios.

Throughout his career, Paris has contributed as a co-inventor on patents, co-author on peer-reviewed publications, and as a stakeholder providing public comments on emerging global regulatory guidelines.

Past Keynote Speakers Each year we feature a keynote speaker for the Department's annual Spring Undergraduate Research Symposium. We are honored to have had speakers who are alumni of the department and are willing to come back and share with our students their experiences of "life after JMU". We thank each of these speakers and look forward to future alumni participation in Spring Symposium.

Year	JMU Class	Speaker	Affiliation
2025	2009	**Dr. Paris Hamilton**	*Agios Pharmaceuticals*
2024	2005	**Dr. Ashley Head**	*Brookhaven National Laboratory*
2023	1994	**Dr. Kevin Bennett**	*Hood College*
2022	1994	**Dr. Timothy W. Graul**	*Pfizer Inc.*
2021	2005	**Dr. Christian Zeigler**	*Vertex Pharmaceuticals*
2019	1995	**Dr. Lisa M. Christianson (M.D.)**	*University of Virginia School of Medicine*
2018	2002	**Dr. William Gemmill**	*Eminess Technologies, Inc.*
2017	2004	**Dr. Zeric Hulvey**	*United States Department of Energy*
2016	2007	**Dr. Reid Gadziala**	*Cleveland Clinic*
2015	1994	**Dr. Michael Leopold**	*University of Richmond*
2014	1996	**Dr. Dana McGraw Dattelbaum**	*Los Alamos National Laboratory*
2013	1999	**Dr. Christy Vestal Martin**	*Vorbeck Materials*
2012	1994 N/A	**Dr. Melissa C. Rhoten** **Dr. Orde Q. Monro**	*Longwood University* *University of KwaZulu-Natal*
2011	1992	**Dr. Morgan S. Sibbald**	*The Sherwin-Williams Company*
2010	1988	**Dr. Kevin Morris**	*Carthage College*
2009	1988	**Dr. Chris E. Holmes**	*The University of Vermont College of Medicine*
2008	1995	**Dr. Jonathan Dattlebaum**	*University of Richmond*
2007	1987	**Dr. Elizabeth Perry (M.D.)**	*Signature Healthcare, Inc.*
2006	1967	**Dr. Carolyn Abitbol (M.D.)**	*University of Miami (FL) School of Medicine*
2005	1975 1976	**Dr. Daniel Downey** **Dr. Gary Rice**	*James Madison University* *College of William and Mary*
2004	1987	**Dr. James (Dusty) Baber**	*National Institutes of Health*
2003	1984	**Dr. Fred King**	*West Virginia University*
2002	1977	**Dr. Roger Bertholf**	*University of Florida School of Medicine*
2001	1979	**Mrs. Katheryn Lam**	*International Business Machines*
1999	1987	**Dr. Jose Madalengoitia**	*University of Vermont*
1997	1986	**Dr. Fred R. Kinder**	*Novartis Research Institute*
1996	1976	**Dr. Terry O. Trask**	*DuPont Chemicals*
1995	1973	**Dr. Carl Lentz**	*Eastman Fine Chemicals*
1994	1990	**Dr. Michele A. Kelly**	*University of Maryland Baltimore County*
1993	1985	**Dr. Cynthia K. Fallon**	*DuPont Chemicals*
1992	1983	**Dr. Laurie Locascio**	*National Institute of Standards and Technology*
1991	1983	**Dr. Noreen Naiman**	*North Carolina School of Science and Mathematics*
1990	1982	**Dr. Matthew T. Stershic**	*Atomchem North Amercia*
1989	1982	**Dr. Michael Kinter**	*Cleveland Clinic Lerner Research Institure*
1988	N/A	**Dr. Thomas J. Meyer**	*Los Alamos National Laboratory*
1987	1980	**Dr. Steven Davis**	*Naval Research Laboratory*
1986	1980	**Dr. Steven A. Hackney**	*Michigan Technological University*
1983	1978	**Dr. Richard B. Lam**	
1982	1975	**Dr. Daniel Downey**	*West Virginia University*
1981	1959	**Mr. Ronald E. Ney**	*Environmental Protection Agency*
1980	N/A	**Dr. Stanley G. Sunderwirth**	*Metropolitan State College (Denver, CO)*
1979	1973	**Dr. Carl Lentz**	*Eastman Fine Chemicals*

Oral Session I: Thursday April 24, 2025 *(King 259)*		
11:00 am	Madeleine Benes, Isabel I. Romov and Dr. Nathan T. Wright	Characterizing Small Molecule/ Desmoplakin Interactions Preventing Protein Degradation
11:15 am	Kamrin D. Shultz, Dr. Callie J. Miller, Dr. Kristopher E. Kubow and Dr. Nathan T. Wright	Roadmap of Obscurin from 2022-2025
11:30 am	Olivia E. Coer and Dr. Brycelyn M. Boardman	Mechanical and Thermal Analysis of Chitosan Films with Polyol-Boric Acid Complexes
11:45 am	Hung Quach, Valeri Krasheninnikov, Tai Quach, Dr. Barbara A. Reisner and Dr. Kevin L. Caran	Synthesis and Characterization of a Novel Polycationic, Hydrophobic, Antimicrobial, Water-Purifying Polymer

Oral Session II: Thursday April 24, 2025 *(King 259)*		
1:00 pm	Joseph C. Loiselet, Mollie M. Corbett, James T. Whitted, Erin D. Schell, and Dr. Ashleigh E. Baber	Monitoring Ethanol Reactivity on a Copper Catalyst with Isotopic Desorption Experiments
1:15 pm	Frances E. Homan, Shyleigh A. Good, Mary M. Sessoms, Carly N. Hemani and Dr Lindsay Caesar	Isolation and Characterization of Secondary Metabolites Induced by Fungal-fungal Co-culture
1:30 pm	Angelina V. Lo Presti and Dr. Christine A. Hughey	Production of Maillard Reaction Intermediates During Mashing and Boiling of a Single Malt, Single Hop (SMaSH) Beer
1:45 pm	Brandy L. Davidson, Nathan Morris, Dr. Brycelyn M. Boardman, and Dr. Gretchen M. Peters	Evaluating the kinetics and thermodynamics of diol-boric acid complexations in organic solvent using NMR spectroscopy
2:00 pm	Lewis D. Crooks IV, Stephanie J. Schwender, Emma J. Goehner, and Dr. Barbara A. Reisner	Dye-ing to Learn: Understanding the Chemistry behind CHEM 132L Water
2:15 pm	Emily M. Euler, Haley E. Frankovich, Dr. Kendra Letchworth-Weaver, and Dr. Ashleigh E. Baber	Surface-mediated Butanol Isomer Selectivity on TiO_2/Au(111) Inverse Model Catalysts

(Student presenters underlined)

Poster Session: Friday April 25, 2025, 1:00 – 3:00 pm *(PCB lobby)*	
Erin Bozman, Ingrid Larne, Jonathan Ryan, Jessica Valle, and Dr. Kevin L. Caran	Synthesis of Biscationic Amphiphiles with Two C_{16} or C_{18} Tails
William Brown, Eric Shepard, Tengis Tamir, and Dr. Debra Mohler	Creation of a Synthetic Strategy for Novel Antisense Oligonucleotide Analogs
Elijah Fernands, Frank Muscarella, Dr. Diana Northup, Dr. Paris Salazar-Hamm, and Dr. Lindsay Caesar	Induction of Secondary Metabolites in Bat-associated Bacteria using SAHA to Fight White-Nose Syndrome
Brian M. Getty, Madeleine Benes, and Dr. Nathan T. Wright	Advancements Towards Characterizing the Desmoplakin-Calpain Interaction
Shyleigh A. Good, Mary M. Sessoms, Frances E. Homan, Carly N. Hemani, and Dr. Lindsay K. Caesar	Induction of Natural Products by Cave Fungal-Fungal Co-cultures
Anna G. Grove, Milan T. Rhodes, and Dr. Gretchen M. Peters	Boronic Acids as Triggerable Units in Supramolecular Gels
Caitlin A. Gutierrez and Dr. Brycelyn M. Boardman	Understanding the Aggregation Induced Emission of Quinazoline Derivatives in the Presence of Glucosamine and Chitosan
James E. Hess, Madison L. Luke, Kiara X. Herrera, and Dr. Christine A. Hughey	Flavor Profiling and Chemical Relationships of Homegrown Vegetables using GC/MS
Elanor Kirkland, Kayla Moore, Dr. Brycelyn Boardman, and Dr. Isaiah Sumner	Molecular Modeling Between Glucosamine and Differing Plasticizers
Elaina X. Manyin and Dr. Isaiah Sumner	Computational Modeling of the Formation of Glycerol Boric Acids Interacting with Glucosamine
Lucille McGinnis and Dr. Nathan T. Wright	Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation
Kayla H Moore and Dr. Brycelyn Boardman	The importance of alcohols: Analyzing the spectroscopic primary and secondary binding interactions between glucosamine, polyols, and glycerol
Stephanie J. Schwender, Aliyah N. Walker, and Dr. Barbara Reisner	Biopolymer-based Methodologies for Adsorption of Metal Contaminants from Aqueous Solutions
Miranda Shackelford, Hayley Larson, and Dr. Gina MacDonald	Investigating the Role of Amino Acids on Protein Stability
Zachary H. Shelor, Dr. Donna S. Amenta, and Dr. John W. Gilje	Synthesis of N-Benzotriazolyl Derivatives as Chelating Ligands for Ruthenium Complexes
Fady Sidarous, Dr. Jonathan Monroe, and Dr. Christopher Berndsen	Structural characterization of the AMY3 catalytic domain
Max Tyree, Max Garcia, Dr. Christine Hughey, Amanda Cicali, Drew Roberts, and Dr. Christine A. Hughey	Variation in the metabolic expression of Ehrlich pathways across brewing yeast strains
Dylan M.Virts, Katelyn Bowers, and Dr. Christine A. Hughey	Identification, Validation, and Quantitation of Unknown Metabolites in SMaSH beer using Molecular Networking

(Student presenters underlined)

Special Announcements: Friday April 25, 2025 *(King 159)*	
3:30pm	Announcement of Chemistry and Biochemistry Student Award Winners

Keynote Address: Friday April 25, 2025 *(King 159)*		
3:35 - 4:35 pm	Paris Hamilton, PhD JMU Class of 2009	Beyond the Lab: Navigating a Career in the Pharmaceutical Industry

Keynote Address

Friday, April 25, 2025 at 3:35 pm
King 159

Beyond the Lab: Navigating a Career in the Pharmaceutical Industry

Paris Hamilton, PhD
(JMU Class of 2009)
Associate Director of Regulatory Affairs
Chemistry, Manufacturing, and Controls (CMC)
Agios Pharmaceuticals
Cambridge, MA

Navigating a career in chemistry is rarely a straight path, and the journey from student to professional can be filled with unexpected twists and turns. In this talk, I will share my personal career journey, from graduating as a chemistry student at JMU to my current role as a regulatory affairs CMC professional in the pharmaceutical industry. Along the way, I'll highlight pivotal moments where I shifted my career focus—starting as an aspiring forensic chemist, then pivoting to synthetic medicinal chemistry, and later transitioning into pharmaceutical R&D and regulatory affairs.

I will discuss the value of staying open-minded and flexible, offering insights into the variety of career options available to chemistry graduates, including research and development, regulatory affairs, policy, consulting, and more. Drawing from my experiences, I will provide practical advice on how to translate the skills gained during a chemistry degree into diverse industry roles. Through this, I hope to encourage students to embrace career pivots and take advantage of the many paths that chemistry can lead to.

By the end of this presentation, students will gain a deeper understanding of the diverse opportunities available in the professional world, while learning how a flexible mindset and curiosity can set them up for success in any field.

STUDENT ABSTRACTS

(Student presenters underlined)

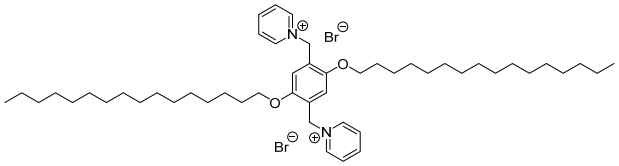
Characterizing Small Molecule/ Desmoplakin Interactions Preventing Protein Degradation

Madeleine Benes, Isabel I. Romov and Dr. Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Mutations in the desmosomal protein desmoplakin (DSP) underlie about 5% of Arrhythmogenic Cardiomyopathy (ACM) cases. Recent data from our lab show that some disease-linked DSP mutations are hypersensitive to calpain, an endogenous calcium dependent protease. The resulting loss of DSP destabilizes the desmosome and leads to weakened cell-cell adhesion, which is correlated with fibrofatty infiltration in ACM. Our lab has probed the molecular mechanism of this DSP degradation, showing that DSP mutant hypersensitivity to calpain is dependent upon the exposure of a usually occluded cleavage site on the DSP surface. Mutant DSP remains folded globally but exhibits increased local dynamics and solvent accessibility around this site. Previous work found that small molecules stabilize DSP levels in the presence of calpain. Several dozen small molecules specifically inhibit DSP and DSP mutant degradation. Here, we continue these studies by showing via STD-NMR that these same drugs bind to DSP at micromolar affinities. In addition, we have begun to characterize the calpain-DSP interaction via SPR and show that these drugs alter this protease-protein interaction. Together, these experiments provide a foundation for future DSP-targeted drug development to prevent ACM.

Synthesis of Biscationic Amphiphiles with Two C_{16} or C_{18} Tails

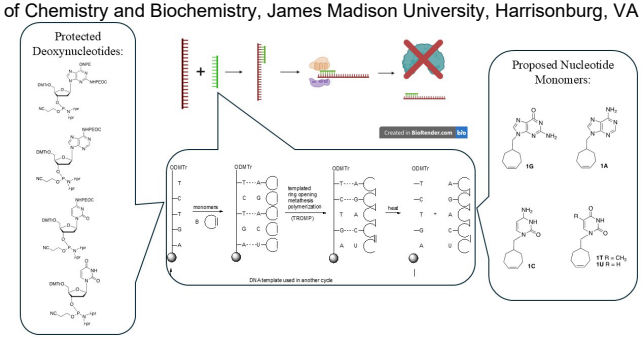
Erin Bozman, Ingrid Larne, Jonathan Ryan, Jessica Valle and Dr. Kevin L. Caran
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Several biscationic, double-tailed amphiphiles are being synthesized in an effort to make novel antibacterial materials. These amphiphiles may prove useful in medical applications where a sterile environment is imperative. Each amphiphile was prepared using a three-step synthesis: (1) Williamson Ether Synthesis, (2) electrophilic aromatic substitution, and (3) Menshutkin reaction. The structure and purity of each isolated intermediate was confirmed using ^{1}H NMR and ^{13}C NMR spectroscopy. Future work includes synthesis of amphiphiles with various headgroups, and colloidal and antibacterial testing.

Creation of a Synthetic Strategy for Novel Antisense Oligonucleotide Analogs

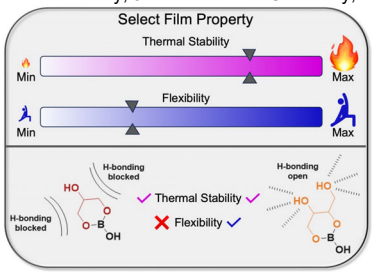
William Brown, Eric Shepard, Tengis Tamir, and Dr. Debra Mohler
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Antisense oligonucleotide analogs (ASOs) are oligomers of around 20 nucleotides that bind to specific sequences of mRNA to prevent the translation of RNA into proteins in gene expression. Although ASOs are highly effective in controlling of proteins production, the do have some limitations. The most consequential of these limitations are the eventual breakdown of ASOs in vivo and the complexity of their synthesis. To address these problems, we propose a novel synthetic strategy for ASOs, in which nucleoside analogs composed of a DNA/RNA base attached ed to a cycloheptene ring undergo a templated polymerization. To synthesize this template, we report the successful preparation of protected deoxynucleoside phosphoramidites This approach will allow for the creation of ASO analogs from nucleoside analog monomers through a one step process.

Mechanical and Thermal Analysis of Chitosan Films with Polyol-Boric Acid Complexes

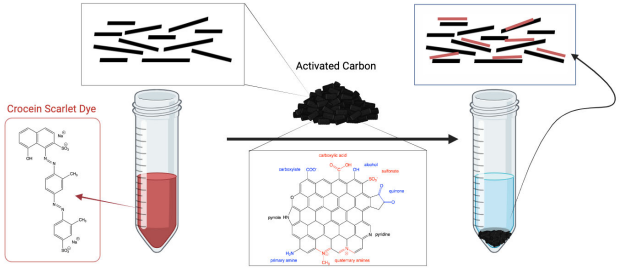
Olivia E. Coer and Dr. Brycelyn M. Boardman
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Chitosan, a natural biopolymer derived from the exoskeletons of crustaceans, is an eco-friendly alternative to petroleum-based plastics that are widely used today. However, optimizing the properties of chitosan materials with plasticizers to fit particular applications remains a significant challenge. Here, we report the ability to control the binding potential of alcohol-rich plasticizers with boric acid. Polyols can form neutral complexes with boric acid (BA) that alter the hydrogen-bonding face of the plasticizer, resulting in changes to the effectiveness of the plasticizer. Glycerol-BA and erythritol-BA systems were previously studied to investigate the impact of increasing the polyol chain from 3 OH to 4 OH units. In chitosan, films with glycerol-BA complexes displayed a decrease in flexibility and an increase in thermal stability, whereas films containing erythritol-BA complexes showed an increase in both thermal stability and flexibility comparatively. Additionally, kinetic analysis of the decomposition was investigated using four different ramp rates in the TGA. Results indicated that polyol concentration is responsible for changes in activation energy and that the decomposition is a complex multistep process. Polyols xylitol, sorbitol, and mannitol containing 5 and 6 OHs respectively were also investigated. Films containing each polyol were prepared with increasing concentrations of BA (0.5 eq - 4 eq). ATR-FTIR, TGA, DSC, and DMA were used to characterize the films. Xylitol-BA-containing films exhibited increased flexibility when compared to erythritol-BA with a decrease in Young's moduli at all concentrations, while the thermal stability was maintained. However, the stereoisomers mannitol and sorbitol do not show the same trends, exhibiting inconsistent behavior with an increase in BA concentration. This may be due to the complex mixture of neutral boron complexes as a result of the increase in polyol length. The combined results demonstrate the ability of BA to modulate the specific hydrogen-bonding interactions between the plasticizer and the polymer.

Dye-ing to Learn: Understanding the Chemistry behind CHEM 132L Water

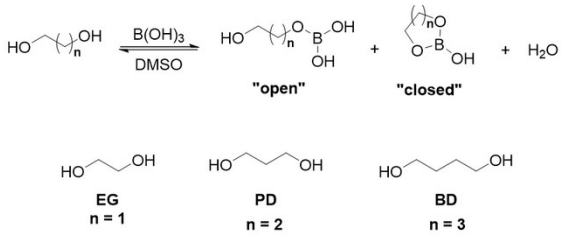
Lewis D. Crooks IV[1], Stephanie J. Schwender[1], Emma J. Goehner[2], and Dr. Barbara A. Reisner[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Chemistry, University of Mary Washington, Fredericksburg, VA 22401



The general chemistry water lab was developed as a research-based lab to better engage students in chemistry and focus on the skills that are critical for scientists and citizens. In this lab, students investigate the adsorption of dyes by activated carbon. The dye-activated carbon system was explored to better understand the factors that affect student results while considering implementation in the general chemistry lab space. The adsorption kinetics of nineteen dyes were studied. Conditions such as tube size and shaking rates were optimized for the lab. Dye uptake is best fit as a two-step process for most dyes and the rate of uptake correlates with dye charge. The adsorption isotherm was determined for crocein scarlet dye and is described by the Freundlich model. The kinetics and thermodynamics of dye adsorption for this lab will be presented.

Evaluating the kinetics and thermodynamics of diol-boric acid complexations in organic solvent using NMR spectroscopy

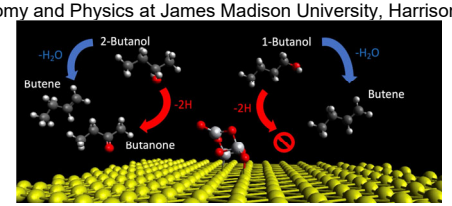
Brandy L. Davidson, Nathan Morris, Dr. Brycelyn M. Boardman, and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Diols are ubiquitous in nature and are common functional groups. The complexation of diols with boric acid (BA) has garnered significant interest due to its ability to form versatile, dynamic networks with unique chemical and physical properties. BA readily forms reversible, covalent B-O bonds with diols, yielding cyclic esters. These diol-BA complexes have broad implications in fields such as drug delivery, materials science, and polymer chemistry. And while this chemistry is well-established in aqueous environments, less is known about the formation of neutral boron complexes with BA in organic solvents. Here, we describe an in-depth NMR spectroscopic study into the complexation of diols with BA to form neutral species in DMSO. Our findings indicate that the diol binding mode impacts both the kinetics and thermodynamics of the complexation reaction. We found that the formation of boron complexes is preferred with 1,3-diols over 1,2- and 1,4-diols, with 1,3-propanediol (1,3-PD) forming approximately three times as much B-O complex as ethylene glycol (EG) and no cyclization being observed with 1,4-butanediol (1,4-BD). The rate of complexation was found to be significantly faster with 1,2-diols than 1,3-diols. While EG forms its neutral boron complex and reaches equilibrium in less than 30 minutes, equilibrium is not reached for 1,3-PD-BA complexes until over 80 hours of mixing. The impact of additional structural variations within the diol have also been explored and significantly impacts the rate and product distribution of diol-BA complexation. When the diols were introduced to a gradual increase in water content, the concentrations of complexes decreased for each diol (1,3-PD, EG, and 1,4-BD). These findings provide important insights into the formation of neutral boron complexes in organic systems and can serve as a model for BA-complexation with more complex diols and polyols.

Surface-mediated Butanol Isomer Selectivity on TiO_2/Au(111) Inverse Model Catalysts

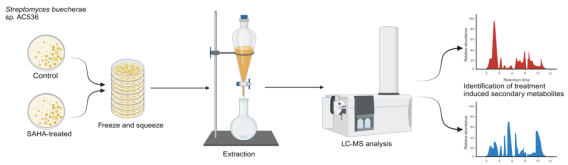
Emily M. Euler[1], Haley E. Frankovich[1], Dr. Kendra Letchworth-Weaver[2], and Dr. Ashleigh E. Baber[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Astronomy and Physics at James Madison University, Harrisonburg, VA 22807



Biofuels such as butanol can be utilized to minimize global fossil fuel reliance while contributing to a carbon-neutral cycle. Biobutanol has low volatility and multiple transportation options which make it an attractive alternative fuel. Understanding the fundamental thermal catalysis processes of butanol over heterogeneous model catalysts can aid in the design of more efficient catalysts. Butanol isomers can be partially oxidized over TiO_2/Au(111) inverse model catalysts, which activate redox reactions of $C_1 - C_3$ alcohols. To better understand the processes in play, temperature programmed reaction spectroscopy (TPRS), atomic force microscopy (AFM), density functional theory (DFT), and high-performance computing are used to investigate its reaction. This study aimed to examine the reactivity of 1- and 2-butanol (BuOH) when exposed to a TiO_2/Au(111) surface. Regardless of TiO_2 coverage, 1-BuOH only formed dehydration products. 2-BuOH formed the dehydrogenation products at low TiO_2 coverages, and at higher TiO_2 coverages formed both the dehydrogenation and dehydration products. AFM images show 1D wirelike nanoparticles of TiO_2 dispersed across the Au(111) surface at low (0.14 ML) coverages. With a higher TiO_2 coverage (0.26 ML) there was an increased size and quantity of nanoparticles. DFT calculations of 1- and 2-BuOH adsorbed on Ti_3O_x nanoparticles supported on Au(111) show two favorable interactions between the butanol and the catalyst material; the oxygen on butanol covalently bonds to the nanoparticle and the alkane chain interacts with the gold surface through dispersion forces. Initial conclusions determine the adsorption energies of both 1- and 2-BuOH to be less dependent on coordination number of the Ti and more dependent on gold surface interactions. These results indicate that there are more active sites available for 2-BuOH to interact favorably with both the nanoparticle and the gold surface compared to 1-BuOH, potentially influencing reactivity and selectivity.

Induction of Secondary Metabolites in Bat-associated Bacteria using SAHA to Fight White-Nose Syndrome

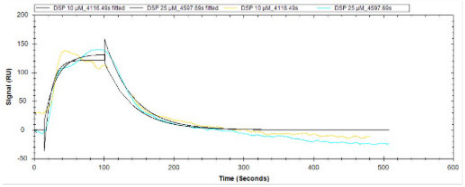
Elijah Fernands[1], Frank Muscarella[1], Dr. Diana Northup[2], Dr. Paris Salazar-Hamm[2], and Dr. Lindsay Caesar[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Biology, University of New Mexico, Albuquerque, NM 87131



Bat populations in North America are in decline due to Pseudogymnoascus destructans, the fungus that causes White-Nose Syndrome (WNS). Over 7 million bats have died in the last decade from this disease, greatly harming ecosystems and agriculture. Fortunately, some caves are still WNS-free, leading scientists to explore how bats living in these caves obtain protection from this disease. In a recent study, 632 bacteria from WNS-free bats were isolated, 36 of which inhibited P. destructans. The antifungal constituents were not identified. Bacteria are sources of valuable bioactive molecules with antimicrobial, antifungal, and anti-inflammatory activities. However, the production of bioactive molecules is dependent on growth conditions, making them challenging to access in a laboratory setting. Bacterial biosynthetic pathways are under strict transcriptional regulation so that energetically expensive products are only formed when they provide a competitive advantage. To maximally activate silent biosynthetic pathways in bat-associated bacteria, we grew twelve bat-associated strains with varying biological activities in the presence of the histone deacetylase inhibitor suberoylanilide hydroxamic acid (SAHA) and evaluated the changes to secondary metabolite production using untargeted metabolomics. In six strains, SAHA led to significant upregulation of secondary metabolites. Using publicly available natural products databases, we have putatively identified 12 molecules that are reproducibly upregulated or completely unique to SAHA-treated cultures.

Advancements Towards Characterizing the Desmoplakin-Calpain Interaction

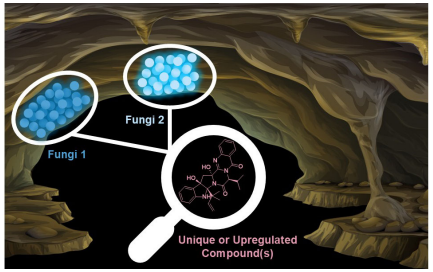
Brian M. Getty, Madeleine Benes, and Dr. Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Desmoplakin (DSP) is a desmosomal protein that plays an integral role in connecting the intermediate filaments from one cardiomyocyte to another. Mutations in DSP underlie about 5% of arrhythmogenic cardiomyopathy (ACM) cases. Recent data from our lab show that some disease-linked DSP mutations result in hypersensitive cleavage in the presence of calpain, an endogenous calcium-dependent protease. The resulting loss of DSP destabilizes the desmosome and leads to weakened cell-cell adhesion, which is correlated with fibrofatty infiltration in ACM. Our lab has shown that DSP mutant hypersensitivity to calpain is dependent upon the exposure of a usually occluded cleavage site on the DSP surface. Previous work found that small molecules stabilize DSP levels in the presence of calpain. Several dozen small molecules specifically inhibit DSP and DSP mutant degradation. Our research implies that there is a binding interaction between DSP and calpain; however, specificities such as binding affinity and preferred conditions are unknown. Here, we begin to characterize the calpain-DSP interaction via SPR and gel electrophoresis. Future work will focus on quantitatively assessing the calpain-DSP interaction and using this data as a comparison to further investigate the possible drug-DSP interactions that could disrupt the calpain-DSP interaction.

Induction of Natural Products by Cave Fungal-Fungal Co-cultures

Shyleigh A. Good, Mary M. Sessoms, Frances E. Homan, Carly N. Hemani and Dr. Lindsay K. Caesar
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Subterranean environments, characterized by extreme conditions, foster the evolution of unique and diverse microbial communities. Among these microbes, fungi are particularly significant for their ability to biosynthesize secondary metabolites (natural products), many of which have found use as drugs, agrochemicals, and more. However, under standard laboratory conditions, many secondary metabolites remain silent. Co-culturing, a technique that involves growing two different fungal strains on the same media, stimulates competition between fungi, potentially activating silent biosynthetic pathways or inducing the production of novel metabolites. On July 3, 2024, six fungal strains were collected from Grand Caverns in Grottoes, VA. Of the possible 15 fungal-fungal co-culture combinations, five were pursued for further study due to visually noticeable interactions in the co-culture as compared to the monocultures. Target co-cultures were prepared for chemical analysis by growing seed cultures on rice, extracting them in $CHCl_3$, and eliminating sugars and fats using liquid-liquid partitioning. The extracts were dried by N_2 and analyzed using untargeted mass spectrometry-based metabolomics. Notable chemical changes, including upregulation of existing metabolites and induction of new compounds, were observed in two of the five co-cultures. Future work will focus on confirming biological reproducibility, identifying the induced compounds through database matching and NMR, and assessing biological activity with assays.

Boronic Acids as Triggerable Units in Supramolecular Gels

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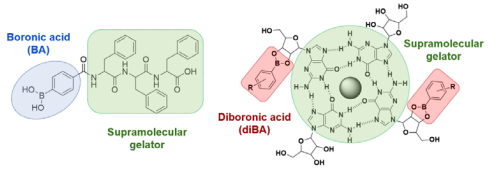

Supramolecular gels have been used for a number of applications, including drug delivery and sensing. These materials are generally biologically compatible and stimuli-responsive, but often lack control and specificity. Boronic acids ($R\text{-}B(OH)_2$, BAs) are useful functional groups capable of forming dynamic, covalent bonds with electron-rich species, such as diols, hydroxide, and fluoride. The incorporation of these units into supramolecular gels introduces novel function and expands their potential applications. Here, we report an exploration into the addition of BAs into supramolecular gels. Two gel systems were investigated: (1) a peptide-based hydrogel with covalently incorporated BA units and (2) a guanosine-based organogel with diboronic acid (diBA) crosslinkers. In both cases, the presence of the BAs aids the gelation process and increases the material stiffness. That is, without a BA unit, both the peptide and guanosine gelators rapidly precipitate under gelating conditions. Additionally, as the concentration of the diBA crosslinker is increased in the guanosine gel, we observe a notable increase in the stiffness of the resulting material. Both gels readily respond to external stimuli, such as pH changes, fluoride, and peroxides. At acidic pH, both the gelators form precipitates. However, as the pH is increased, self-supporting gels form until the concentration of hydroxide is in excess, at which point free-flowing solutions are observed. Fluoride and peroxides both readily bind to boron, resulting in material changes in the peptide gel. Peroxides also rapidly reacts with the gelator molecules, breaking the C-B bond. The free BA units within peptide-based hydrogels can be also used to incorporate diol-based drugs and dyes, indicating this material could be a useful drug delivery system. These findings highlight the implications of using BAs in supramolecular gels. In the future, we will explore light-sensitive diBA crosslinkers and the use of these materials for drug delivery and environmental clean-up.

Understanding the Aggregation Induced Emission of Quinazoline Derivatives in the Presence of Glucosamine and Chitosan

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Amine sensing bio-plastics are potentially powerful materials that can help solve the food and plastic waste crises simultaneously. Quinazoline derivatives, acetylated 2-(2-hydroxyphenyl)quinazolin-4(3H)-one (HPQ-Ac) and 2-(2-hydroxyphenyl)quinazolin-4(3H)-one (HPQ) have previously been studied as amine sensors. In the presence of amine vapor, HPQ-Ac is converted to HPQ, which promoted aggregation-induced emission (AIE) in the HPQ turning the sensor to the “on” state. HPQ-Ac was incorporated into chitosan films, however these films fluorescence in the absence of amine. To further investigate the lack of an “off” state of the sensor in these materials, glucosamine (GlcN), the repeat unit of chitosan, was used as a model system. Fluorescence and nuclear magnetic resonance (NMR) spectroscopy were used to investigate these interactions. NMR titration experiments were performed in d-DMSO holding the concentration of HPQ or HPQ-Ac constant while increasing the concentration of GlcN. In a similar experiment HPQ or HPQ-Ac and GlcN are held constant and the concentration of glycerol is increased, both quinazoline derivatives display a similar trend in which their interaction with GlcN is reduced. Fluorescence experiments were then performed on the systems investigated in the NMR. AIE was not observed for HPQ-Ac with increasing concentration of GlcN in H2O/THF but an increase in emission intensity was observed in DMSO. As was observed in the NMR experiments, the addition of Glyc had little impact on the system, showing no changes in emission intensity with increasing concentration of glycerol. Chitosan solutions containing HPQ-Ac were also investigated, AIE is clearly observed but can be reduced by decreasing the concentration into the micromolar range. The model system has elucidated that there are strong interactions between HPQ-Ac and GlcN which are likely the cause of the observed AIE in the chitosan films. Films with reduced concentration of HPQ-Ac are currently being investigated.

Flavor Profiling and Chemical Relationships of Homegrown Vegetables using GC/MS

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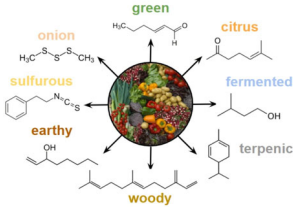

Volatile organic compounds (VOCs) responsible for the taste and aroma of foods are called flavor compounds. In this discovery-based study, solid phase microextraction gas chromatography-mass spectrometry (SPME GC/MS) was used to profile flavors in 33 different vegetables and herbs harvested from a backyard garden between May and July 2023. Several different sample preparation methods were explored. The best method chopped/grated, lyophilized and powdered the samples. Each sample contained 0.25 g of powdered vegetable/herb and was spiked with an internal standard (1000 ppm ethyl Hexanal-d12 in MeOH), equilibrated in a 40 °C water bath for 15 min, and then transferred to a 40 °C hot plate for 30 min. A DVB/Carbon WR/PDMS SPME Arrow fiber was exposed to the headspace of the sample for 30 min whilst the sample was stirred and heated on the hot plate. The adsorbed compounds were thermally desorbed from the fiber in the GC inlet for 3 min. The compounds were separated on a DB-5 GC column and identified by comparing mass spectra to the NIST library. Data were imported into Mass Profiler Professional, filtered by abundance (200000 - 7459225), and evaluated based on the flavor compounds identified and each vegetable's assigned biological family. The number of compounds detected in the samples ranged from 1 in the little gem lettuce, shell of a green pea, and pepperoni pepper to 33 in the dill out of 74 compounds total compounds. The number of observed compounds is low due to the high abundance threshold used. Hierarchical clustering revealed some clustering by biological family. Data was also visualized in a molecular network using GNPS Molecular Networking program which allowed for more clarity visualizing the family's relationships and their related compound clusters. A total of 230 unique compounds were identified in the samples through molecular networking. This work demonstrates the use of two untargeted metabolomic approaches to flavor profiling.

Isolation and Characterization of Secondary Metabolites Induced by Fungal-fungal Co-culture

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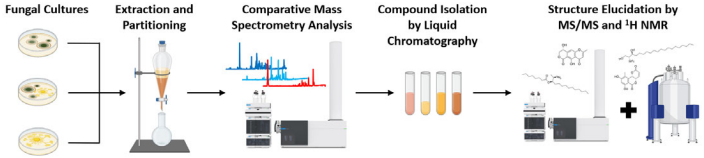

Fungal natural products, also known as secondary metabolites, have played a major role in pharmaceutical and agrochemical development. In fungi, secondary metabolites are produced by biosynthetic gene clusters (BGCs), which consist of one or more backbone enzymes, tailoring enzymes, and sometimes a transcription factor that regulates their expression. However, the majority of fungal BGCs remain silent under laboratory conditions and their associated metabolites are not produced unless induced by an external stressor. The technique of co-culturing, in which two or more fungal strains are grown on the same media to introduce competition for limited space and resources, has been shown to induce the expression of silent BGCs that form secondary metabolites not found in monoculture. Nine fungal strains were isolated and grown from soil in Harrisonburg, VA and a tenth strain was collected from Grand Caverns in Grottoes, VA. Fourteen of the 45 possible fungal-fungal co-cultures were pursued for further study due to visual changes in the appearance of the fungi in the co-culture as compared to the monoculture. Target co-cultures were prepared for chemical analysis by growing cultures on rice and subjecting them to chemical extraction and liquid-liquid partitioning. The resulting extracts were analyzed using mass spectrometry-based metabolomics. Abundant chemical changes were witnessed in a subset of five co-cultures; one of the five co-cultures showed consistent reproducibility of upregulated metabolites and has been prioritized for targeted study. Two of the four major upregulated compounds produced by this co-culture have been tentatively identified using mass spectrometry and publicly-available natural products databases. The purification of the four upregulated target metabolites by HPLC is in progress and existing chemical databases, MS/MS fragmentation data, and ^{1}H NMR will be used for structure elucidation.

Molecular Modeling Between Glucosamine and Differing Plasticizers

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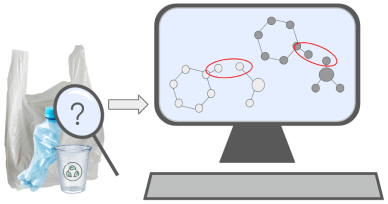

Currently, plastic is commonly made up of petroleum-based synthetic polymers that are detrimental to the environment, in part because they do not decompose. Because plastic is an extremely valuable material, it is critical to find a way to create a more environmentally friendly plastic. Bioplastics may provide a solution. One bioplastic is formed from chitosan – an abundant biopolymer derived from chitin found in the exoskeleton of arthropods – and a plasticizer – an additive that can change the physical properties of chitosan. Currently, the molecular interactions between the chitosan and the plasticizer and how they affect the bioplastic's properties are not well understood. Therefore, we have previously performed computational experiments to quantify the interactions between D-glucosamine (the base unit of chitosan), and several polyol plasticizers (glycerol, 1,2-propanediol, 1,3-propanediol, and ethylene glycol). However, D-glucosamine has two, naturally occurring isomers: α and β. Chitosan is made of the β isomer, and previous work used the α isomer. So, this work focuses on the interactions between β-D-glucosamine and polyol plasticizers. To understand the molecular-level interactions between these diols and glucosamine, and to find the most stable structures, optimization and frequency calculations were run using the M06-2x density functional combined with two basis sets: 6-31+G(d) and 6-311+G(2d,p). The experiments found that the diols (1-2-propanediol, 1-3-propanediol, and ethylene glycol) seem to drive glucosamine aggregation, in agreement with previous results. Finally, the difference in energy between rotational isomers of the diols was calculated, to help interpret experimental data, which suggests each diol has a different hydrogen-bonding propensity.

Production of Maillard Reaction Intermediates During Mashing and Boiling of a Single Malt, Single Hop (SMaSH) Beer

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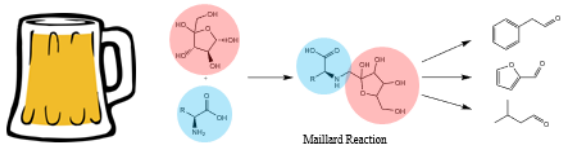

The Maillard reaction is a non-enzymatic reaction that occurs between reducing sugars and amino acids in the presence of heat to produce a variety of compounds that impact the color and flavor of beer. This reaction has predominantly been studied in the kilning of malt. Here we investigate the Maillard reaction during the mashing and boiling of a single malt, single hop (SMaSH) beer and in laboratory-scale brewing experiments. Samples collected throughout mashing and boiling of the SMaSH beer revealed the presence of Amadori rearrangement products (ARPs) and Strecker aldehydes–both important intermediates in the Maillard reaction. The rapid increase of 3-methylbutanal at the end of boiling suggested that these reaction intermediates were produced during mashing, not just being extracted from the malt. To test this hypothesis, laboratory-scale brewing experiments were conducted with a 2:1 ratio of maltose to amino acid (either leucine, Leu, or phenylalanine, Phe). The solution was heated for 60 minutes at 90°C followed by 60 minutes at 105°C while a constant volume was maintained. Amino acids and ARPs were quantified using HILIC positive-ion LC/MS-QqQ-MS. MS/MS experiments were performed on ARPs using q-TOF MS, and fragmentation patterns of ARPs were confirmed by matching to the literature. Maltose was also quantified using a HILIC method in negative ion QqQ-MS while volatile flavor compounds were quantified with headspace solid phase microextraction (HS-SPME) GC/MS. ARPs increased significantly after 60 minutes of heating in both Leu and Phe systems. Flavor compounds also increased. The Phe system saw an increase in phenylacetaldehyde while the Leu system saw an increase in 3-methylbutanal across mashing and boiling. Accordingly, amino acid and sugar concentrations decreased. Thus, laboratory experiments confirm that ARPs and their respective flavor compounds are produced during brewing and likely contribute to the color and flavor of the final beer.

Monitoring Ethanol Reactivity on a Copper Catalyst with Isotopic Desorption Experiments

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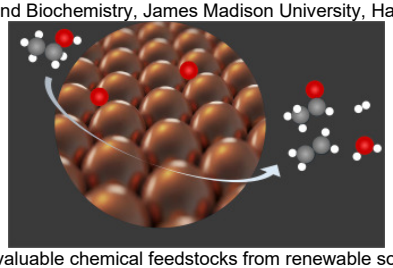

Exploring the formation of valuable chemical feedstocks from renewable sources is critical for decreasing global dependence on fossil fuels. The decomposition of ethanol forms acetaldehyde, a solvent and precursor for dyes, pesticides, pharmaceuticals and more; ethylene, which is crucial for the plastics industry; and clean hydrogen, a necessity for all hydrogenation reactions. While it is well known that Cu(111) and oxidized Cu(111) catalyze the dehydrogenation of small primary alcohols to form aldehydes, dehydration products to form alkenes are less discussed. An in depth study of the reactivity of ethanol on O/Cu(111) shows dehydrogenation, dehydration, and combustion products using temperature programmed reaction spectroscopy (TPRS). The presence of oxygen on O/Cu(111) resulted predominantly in acetaldehyde formation via the dehydrogenation pathway, with lesser amounts of ethylene via dehydration, as well as combustion products. Successive TPRS experiments resulted in decreased yields of all products due to the consumption of surface oxygen via water formation <200 K. Isotopic studies of ethanol–OD indicate the role of the hydroxyl hydrogen in water formation from Oads compared to water that desorbs during dehydration, as well as hydrogen formation via the dehydrogenation pathway. The dehydration pathway is proposed to occur via autocatalytic production of Oads during the ethoxy transformation to ethylene, furthering the reaction to form ethylene and CO_2.

Computational Modeling of the Formation of Glycerol Boric Acids Interacting with Glucosamine

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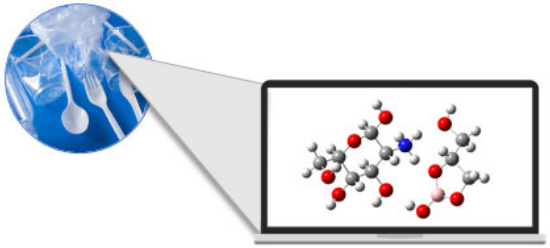

A biodegradable plastic is formed from chitosan, which comes from crustaceans' shells, combined with plasticizers. In a recent set of experiments, borate esters with glycerol were used as plasticizers. Although this combination resulted in poor plasticity, borate ester plastics are stiff and thermally stabile. To understand the molecular interactions that lead to these properties, computational experiments were run to examine the interactions between β-D-glucosamine (the repeat unit of chitosan) and glycerol boric acids (1,2-glycerol boric acid or 1,3-glycerol boric acid). Density functional theory (DFT) at the M06-2X/6-311+G(d,p) level-of-theory showed glucosamine interacts more strongly with 1,2-glycerol boric acid. Furthermore, important IR stretches were identified to assist in experimental IR analysis. Specifically, the H-N-H bends around 1620-1680 cm^{-1}, B-O stretches (1000-1500 cm^{-1}), B-O-H bends (995-1300cm^{-1}), and out of plane boron stretches (600-700cm^{-1}) are clear, identifying peaks. Finally, ΔGs of reaction for the formation of the borate esters (1,2-glycerol boric acid, 1,3-glycerol boric acid, 1,2-propanediol boric acid, and 1,3-propanediol boric acid) from boric acid and different polyols were calculated to explain experimental yields. Our calculations show that intramolecular hydrogen bonds play a key role in stabilizing both reactants and products. Alongside these results, current calculations are being run to explore reaction barrier heights and to explain experimental yields for the synthesis of erythritol boric acids.

Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation

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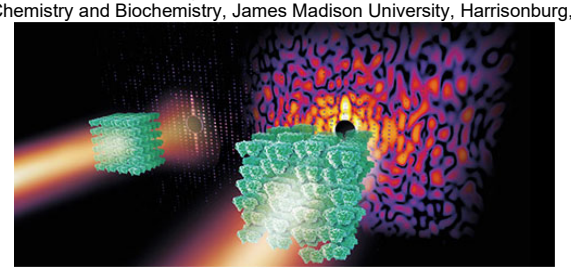

Desmoplakin is a protein in the desmosome that plays an integral role in connecting the intermediate filaments from one cardiomyocyte to another. Some desmoplakin mutations have been linked to arrhythmogenic cardiomyopathy and fragile skin disease. Specific mutations in DSP (R451G, S507F, S442F, and S299R) result in hypersensitive cleavage in the presence of the protease calpain. To block this cleavage event, we have screened drugs for their ability to specifically inhibit calpain-dependent DSP degradation. STD-NMR experiments further confirm that 12 of the drugs bind to DSP in the uM range. Here we begin studies designed to interrogate where the most promising drugs bind to desmoplakin, using biomolecular crystallography experiments.

The importance of alcohols: Analyzing the spectroscopic primary and secondary binding interactions between glucosamine, polyols, and glycerol

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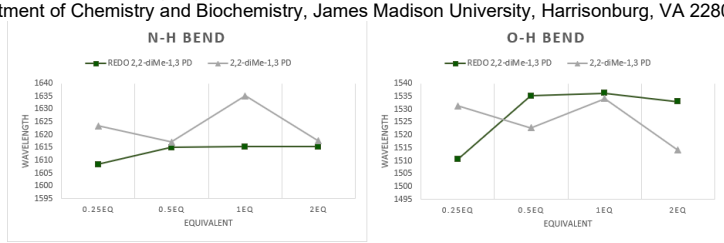

The use of bioplastics as alternatives to petroleum-based plastics has gained significant attention in recent years. These biomaterials are typically created by combining biopolymers like chitosan with plasticizers such as glycerol (Glyc). Previous research has shown that the amount and type of alcohol used can significantly affect the polymeric structure. Chitosan's repeat unit, glucosamine (GlcN), and Glyc are key compounds in forming polyol solutions. Glycerol can have primary binding sites (1,2 or 1,3-OH) and secondary binding interactions due to its additional hydroxyl groups. To explore the impact of primary binding on GlcN aggregation, ethylene glycol and (1,3)-propanediol were used to probe the 1,2 and 1,3 binding modes. Various diols, including (1,2)-propanediol, (2,3)-butanediol, and (2,4)-pentanediol, were analyzed to understand secondary binding while keeping primary interactions constant. This summer, additional polyols such as 2-methyl-(1,3)-propanediol, 2,2-dimethyl-(1,3)-propanediol, (1,2,4)-butanetriol, 2-(hydroxymethyl)-(1,3)-propanediol, 2-(hydroxymethyl)-(1,4)-butanediol were tested to evaluate how an increased alcohol content affects GlcN aggregation and disaggregation. Spectroscopic techniques, including dynamic light scattering (DLS), attenuated total-reflectance infrared spectroscopy (ATR-IR), and nuclear magnetic resonance (NMR), were used to analyze the intermolecular interactions between these diols and GlcN. While most of the analysis focused on ATR-IR, solutions of polyols like Xylitol, Sorbitol, and Mannitol were compared to diols and triols to assess their impact on binding and aggregation. Results indicate that a higher alcohol content leads to increased hydrogen bonding at the molecular level, with more significant hydrogen bonding observed in polymeric chitosan solutions than in glucosamine solutions.

Synthesis and Characterization of a Novel Polycationic, Hydrophobic, Antimicrobial, Water-Purifying Polymer

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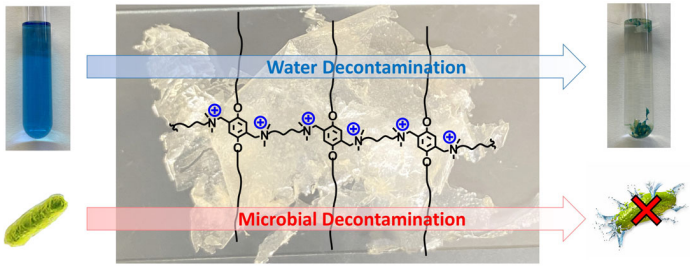

A polycationic, hydrophobic polymer was prepared in four synthetic steps in an effort to develop novel antibacterial materials, capable of decontaminating water. The design of the polymer is based on antibacterial polycationic amphiphiles previously studied in our lab. In the final synthetic step, a bis-electrophile [1,4-bis(bromomethyl)-2,5-bis(hexadecyloxy)benzene] and a bis-nucleophile [1,12-bis(dimethylamino)dodecane] were combined in a Menshutkin polymerization. End-group analysis (^{1}H NMR) was used to estimate the average length of the polymer. AFM and thermal studies were conducted to study the physical properties of the polymer. Dye absorption studies demonstrated the polymer's capacity to selectively remove anionic organic impurities from water. Future work will include exploring the polymer's potential as a novel coating to render surfaces antibacterial.

Biopolymer-based Methodologies for Adsorption of Metal Contaminants from Aqueous Solutions

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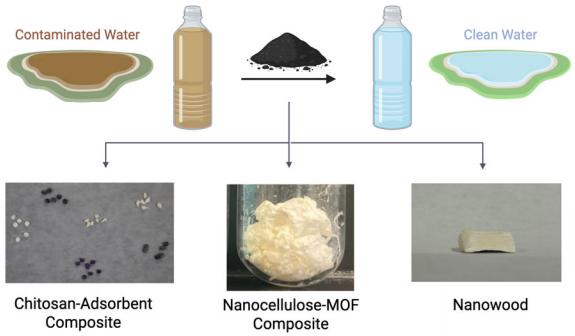

Biocomposites are promising materials for the selective adsorption of metal contaminants from aqueous systems. Multiple biopolymers were investigated to fabricate a structurally stable material with high ion adsorption capacity. Nanocellulose-metal organic framework (MOF) composites, chitosan-adsorbent (MOF, graphene, activated carbon) composites, and nanowood were explored. The nanocellulose and chitosan composites were synthesized from a gel, then a ligand and metal salt or carbon adsorbent were added to form the composite. The nanocellulose and chitosan composites were freeze-dried to form a solid aerogel. Powder X-Ray diffraction (PXRD) and Infrared (IR) spectroscopy data were collected to understand the structure and chemical composition of the resulting materials. Nanowood was prepared by the delignification of balsa wood using sodium hypochlorite. Dye uptake of chitosan composites and nanowood was studied using UV-Vis spectroscopy. The limitations of the biomaterials and their adsorption capacities will be discussed.

Investigating the Role of Amino Acids on Protein Stability

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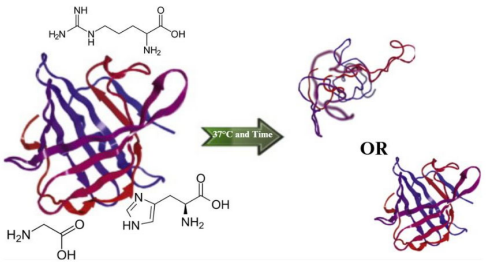

Understanding environmental influences on protein stability is crucial for understanding the mechanisms underlying degenerative neurological diseases. This study aims to investigate the impact of environmental conditions, specifically the presence of various amino acids, on the stability and unfolding of proteins. The model proteins used for study were Beta-Lactoglobulin (BLG) and Beta Serum Albumin (BSA). Infrared spectroscopy was used to monitor protein structure and stability over several weeks. Proteins were incubated with various amino acids including Histidine, Arginine, and Glycine to determine if the amino acids altered protein structure over time as compared to proteins in the absence of amino acids. Our results suggest that all of the amino acids destabilized BLG over time. However, the control BSA was generally more stable over time and only Histidine and Glycine destabilized BSA. These findings suggest that amino acid interactions differentially impact protein stability and underscores the necessity for further research to elucidate these mechanisms.

Synthesis of N-Benzotriazolyl Derivatives as Chelating Ligands for Ruthenium Complexes

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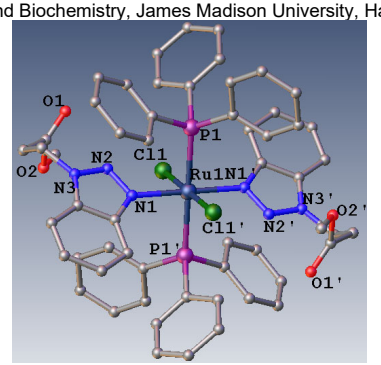

In this study we are preparing and studying the asymmetric (L1) and symmetric (L2) isomers of N-benzotriazolylpropanoate, and their corresponding carboxylates. These are potentially hemilabile ligands that can coordinate to a metal through a heterocyclic nitrogen and/or an oxygen in the ester or carboxylate moiety. The solvent-free, catalyst-free Michael addition of benzotriazole with methylacrylate resulted in the formation of esters L1 and L2. These isomers were separated by elution chromatography and allowed to react with tetrabutylammonium hydroxide (TBAH) to form the corresponding carboxylate anions. These anions, denoted as L3 and L4, were characterized using NMR and IR spectroscopy. Each of these carboxylates was allowed to react with dichlorotris(triphenylphosphine) ruthenium(II), [RuCl2(PPh3)3], and the products were investigated with 31P NMR spectroscopy. These data indicate that the reaction yielded multiple products, which have yet to be separated and individually characterized. Treatment of L2 with [RuCl2(PPh3)3] in toluene at 80℃ showed no reaction. Reaction of L1 in room temperature acetone with [RuCl2(PPh3)3] yielded complex 1. Complex 1 has been characterized by 31P NMR, IR, elemental analysis, and single crystal X-ray analysis. The possible rearrangement of Complex 1 in solution is currently being investigated.

Roadmap of Obscurin from 2022-2025

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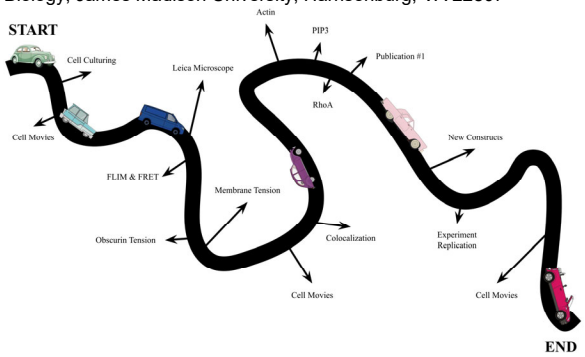

Obscurin is a large modular cytoskeletal protein with multiple signaling domains. While it is most highly expressed in myocytes, obscurin is also the second most mutated protein in breast and colorectal cancers and is significantly downregulated in pancreatic cancer. Obscurin derives its oncogenic properties, at least in part, through its ability to modulate cellular motility and migration; obscurin knockdown in cultured cells leads to increased migration and the start of the epithelial-to-mesenchymal transition (EMT). While it hasn't been definitively proven, obscurin likely controls cell motility through the obscurin RhoGEF domain interaction with the RhoA/ROCK pathway and/or the obscurin PH domain interaction with a PI(3)K/PIP3 pathway. Here, we explore both pathways in more depth. We find that obscurin localizes to the membrane. Obscurin-expressing MDCK cells are largely nonmotile. Cells containing a ΔPH obscurin construct display normal PIP3 levels yet show decreased motility. Cells with ΔRhoGEF obscurin construct, while expressing normal RhoA activity, also show decreased motility, suggesting that both pathways are sufficient to hinder cell migration and both pathways work independently of each other. Both the actin cytoskeleton and overall membrane tension are compromised in cells expressing obscurin, which likely partially accounts for the decrease in migration speed. In total, obscurin's subcellular location and specific downstream targets exhibit a redundant mechanism of cell motility control.

Structural characterization of the AMY3 catalytic domain

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The alpha amylase AMY3 from Arabidopsis thaliana plays a role in starch metabolism and the response to stress. The structure and regulation of AMY3 remain poorly understood. Previous work suggested that AMY3 has three domains: the CBM domain, which binds to carbohydrates, the alpha-alpha hairpin which is a protein-protein interaction domain, and the amylase domain which is responsible for the degradation of the starch polymer. To describe the catalytic function of AMY3 in more detail, we expressed and purified the catalytic domain of AMY3. We then performed small-angle X-ray scattering (SAXS) to describe the structure, showing that the protein was a globular, monomer. AMY3 is known to dimerize and can form disulfides, however it is not clear whether it is an intra- or intermolecular interaction. We carried out copper crosslinking experiments to form disulfides. Our results showed clear evidence of intermolecular disulfide bond formation under oxidizing conditions. Current work is aimed at determining the structure of this dimer. This suggests that AMY3 can respond structurally to changes in the redox environment. Together, SAXS and crosslinking data provide a first look at the structural dynamics of plant AMY3. These findings may inform future studies on how AMY3 functions during plant stress responses and starch metabolism.

Variation in the metabolic expression of Ehrlich pathways across brewing yeast strains

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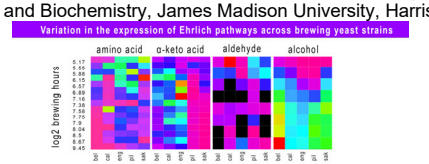

Metabolic processes that occur during fermentation largely impact the flavor profile of the final beer. Our group uses targeted and untargeted metabolomic techniques, along with the coupling of GC/MS and LC/MS data, to better understand flavor development during beer brewing and fermentation. Here targeted metabolomics was used to monitor metabolites formed in the Ehrlich pathway during fermentation of a single malt, single hop (SMaSH) pale ale with five genetically different yeasts, including a Belgian Saison, a California ale, a Czech pilsner lager, an English ale, and a Sake. In the Ehrlich pathway, yeast converts branched and aromatic amino acids to aldehydes and fusel alcohols. We monitored the Ehrlich pathway by collecting samples every 12 to 24 hours throughout fermentation. The volatile metabolites were quantified by use of SPME GC/MS. The amino acids were quantified by HILIC (+) ESI q-TOF MS. Intermediates, such as alpha-keto acids, were observed in either (+) or (-) ESI reverse phase LC q-TOF MS data. The identities of intermediates was confirmed by MS/MS and matching to authentic standards. By monitoring the respiration rate of each fermentation tank, it was clear that the metabolic rates of yeasts differed, likely because they were fermented under identical conditions and not the ideal conditions of each strain. The Czech Pilsner, the only lager yeast studied, produced CO2 bubbles much later than the ales. This difference in metabolic rates was reflected in the decrease in concentration of the amino acids, and subsequent production of the alpha-keto acids and fusel alcohols. For example, the Belgian Saison produced the highest concentration of 2-and 3-methyl butanol from isoleucine and leucine, respectively; while the California and English ales produced these flavor compounds at the lowest concentrations. The Belgian Saison also produced 2-phenylethanol, which arises from phenylalanine, at the highest concentration. The development of these flavors, and others, will be displayed as heat maps to show the progression of flavor development by genetically different yeast strains throughout fermentation.

Identification, Validation, and Quantitation of Unknown Metabolites in SMaSH beer using Molecular Networking

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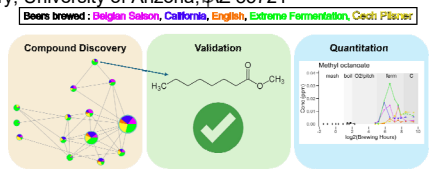

Beer is a complex mixture of volatile and nonvolatile compounds that arise from malt, hops, and fermentation. A pale ale wort brewed from a 2-row malt and Cascade hops was equally divided and fermented with five genetically different yeast: WLP 001 California Ale, WLP 002 English Ale, WLP 566 Belgian Saison, WLP 800 Czech Pilsner Lager, and Wyeast 4347 Extreme Fermentation. Previous work used solid phase microextraction (SPME) and gas chromatography/mass spectrometry (GC/MS) to quantify known flavor compounds. That data set was then placed into Global Natural Product Social (GNPS) to make a molecular network in order to identify new flavor compounds. Molecular networks are composed of compounds with similar mass spectra. Compounds were tentatively identified by comparing their mass spectra to freely available GC/MS libraries. Eighteen compounds matched the library spectra well enough that analytical standards were purchased. By matching mass spectra and retention times of the purchased compounds to the beer samples, six flavor compounds were validated: methyl octanoate, methyl decanoate, methyl dodecanoate, styrene, isoamyl decanoate, and ethyl lactate. After validation, internal calibration was performed to quantify the amount of flavor compound throughout brewing and fermentation. It was found that all these compounds were produced during fermentation, but their concentration differed across yeast strains. Styrene only appeared in the belgian yeast strain. Methyl dodecanoate, methyl octanoate, and isoamyl decanoate were most concentrated in the extreme fermentation strain while the concentration of methyl decanoate was about equal in belgian and the extreme fermentation yeasts. Ethyl lactate was most concentrated in the pilsner strain. This research will help brewers' identify what yeast strain they wish to use as it will give them a better idea on the flavor and aroma profile of each yeast.

Atomic Scale Imaging of Carbon Precursors to Graphene Growth on Ni(111)

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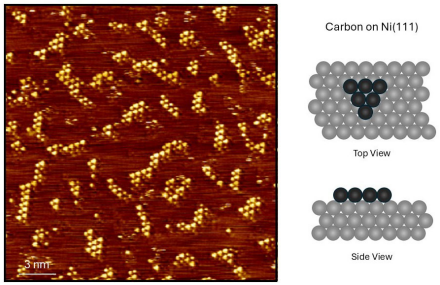

Graphene is a vital resource in developing modern nanofabrication processes and energy storage devices. Witnessing the formation of graphene on Ni(111) is integral to understanding the mechanism for graphene growth. Ni(111) is highly reactive for carbon deposition and growth, which is both good and bad. There is capability for abundant graphene production, but it is thermally selective and difficult to suppress. Following the Boudard reaction ($2CO \rightarrow CO_2 + C$), carbon is observed on Ni(111) in two forms: graphene on terraces and nickel carbide on step edges. Low temperature scanning tunneling microscopy (STM) was used to image the atomic structures of carbon on Ni(111). MountainSPIP was used to process and analyze the images collected via STM, revealing the hexagonal formation of C atom graphene precursors, patches of hexagonal graphene, and square packed carbide structures on the Ni(111) surface. These images show the dynamic nature of carbon on Ni(111) at temperatures as low as 9 K as well as the atomic structure of graphene carbon precursors. Atomic scale images are critical for revealing the mechanisms for graphene growth on solid surfaces.

Exploring the Epoxidation of Isoprene on Copper-Based Catalysts

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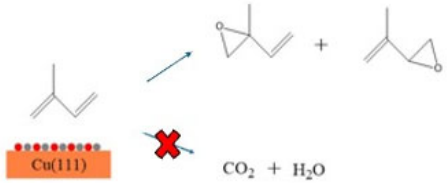

Isoprene (C_5H_8) is a common greenhouse gas that forms the infamous haze observed over the Blue Ridge Mountains. It contributes to a large portion of the planet's ozone formation, and therefore finding alternative value-added uses for isoprene is critical. Isoprene is a diene and has both allylic hydrogen and non-allylic hydrogen sides. It is therefore a model reactant molecule for studying selective epoxidation. Atomic oxygen on Cu(111) is known to enhance the epoxidation of propylene, which contains allylic hydrogens, while Ag(110) and Ag(111) with atomic oxygen encourages the epoxidation of ethylene, which does not have allylic hydrogens. This molecule is ideal to study epoxidation reactivity on a AgCu near surface alloy (NSA), specifically for its allylic hydrogen and non-allylic hydrogen sides, which mimic propylene and ethylene. Creating an NSA comprised of Ag atoms on Cu(111) is expected to produce a favorable surface to form an epoxide from isoprene, while also limiting the unwanted combustion pathway. Ultra-high vacuum temperature programmed desorption (UHV-TPD) spectra were gathered on clean and partially oxidized Cu(111) and Ag/Cu(111) after dosing isoprene. As the amount of oxygen dosed on Cu(111) increased, carbon dioxide yield also increased, indicating that the combustion pathway was in full effect. To minimize overoxidation of isoprene to CO2 under UHV, Ag was deposited on Cu(111) via physical vapor deposition. Auger electron spectroscopy was used to determine Ag coverages on the surface, post-deposition. TPD results indicate that the combustion pathway was deterred in the presence of 1 ML of Ag/Cu. Future work will focus on potential coexisting products and the molecular geometry of isoprene adsorption and packing using scanning tunneling microscopy.

2025 Department of Chemistry and Biochemistry Student Award Winners

D.S. Amenta Award	Anna G. Grove
R.D. Cool Award	Nathan E. Morris
J.W. Chappell Scholarship (May 2024)	Emily N. Davidson
Palocsay Award in Undergraduate Research (2024)	Tengis Tamir
Deborah Warnaar & Brian F. Bauer Chemistry Scholarship (2024)	Daphne M. Antwi
Barbara Pamplin Shell Scholarship in Chemistry (2024)	Anna G. Grove
Service Award	Angelina V. Lo Presti
J. W. Chappell Award	Josephine M. Swanton
American Institute of Chemists	Haley E. Frankovich
Degesch America Award	Frances E. Homan
ACS Award	Shyleigh A. Good
Liberty Casali Memorial Scholarship Fund (2024)	Eric J. Shepard
Dean's Award (Chemistry)	Angelina V. Lo Presti
Dean's Award (Biophysical Chemistry)	Isabella M. Daniel
CRC First Year Student Award	Kayla S. Cote
NOBCChE Dr. Iona Black Award	Caitlin A. Gutierrez
Inclusive Excellence Award	Kayla H. Moore
Phi Beta Kappa Inductee	Peter R. Henry
Outstanding Student Researcher Award	*to be announced*

Divisional Awards

ACS Analytical Award	Angelina V. Lo Presti
ACS Biochemistry & Chemical Biology Award	Angelina M. Sardelli
ACS Environmental Award	Evelyn L. Haugh
ACS Inorganic Award	Zachary H. Shelor
ACS Organic Award	Eric J. Shepard
ACS Physical Award	Joseph C. Loiselet

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