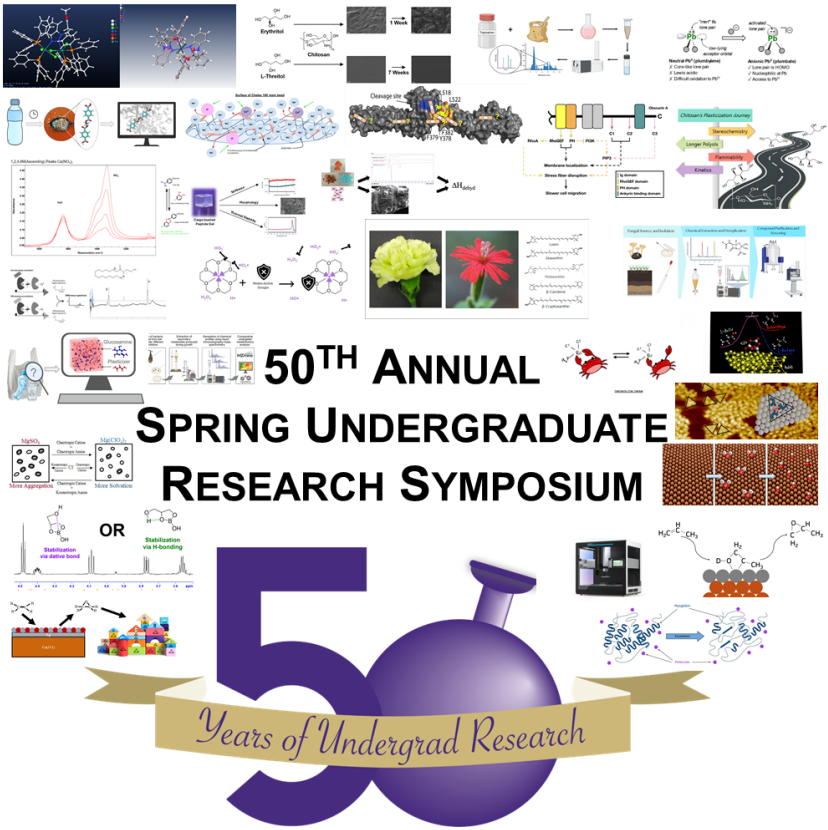
JAMES MADISON UNIVERSITY.

DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY



THURSDAY APRIL 23, 2026

ORAL SESSION I: 10:00AM – 11:15AM (KING 259)
ORAL SESSION II: 1:30 – 2:30PM (KING 259)

FRIDAY APRIL 24, 2026

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

50th Annual Department of Chemistry and Biochemistry
Spring Undergraduate Research Symposium

Keynote Speaker

Jeff Keister, PhD

(JMU Class of 1993)

Deputy Division Director, Data Science and System Integration
National Synchrotron Light Source II
Brookhaven National Laboratory
Upton, New York

Jeff Keister is Deputy Division Director for Data Science and System Integration (DSSI) at the National Synchrotron Light Source II (NSLS-II) of Brookhaven National Laboratory (BNL). He graduated from James Madison University with a B.S. in Chemistry in 1993. During his time at JMU, Jeff performed unimolecular decomposition research with Tom DeVore, catalysis research at Clemson University, and gas-phase laser research at Georgia Tech.

After graduating from JMU, Jeff studied gas-phase ion dissociation at UNC Chapel Hill, performing experiments in the lab as well as at synchrotrons in Berkeley and Paris, before completing his Ph.D. in 1997. Afterwards, Jeff served as a National Research Council fellow for the Army Research Office, conducting research at North Carolina State University and making regular measurements of silicon surfaces and interfaces at the NSLS on Long Island, New York. Starting in 2000, Jeff worked at KLA Instruments, supporting development and application of patterned wafer inspection equipment for semiconductor manufacturing. In 2004 he returned to NSLS to run beamlines for a consortium of users requiring absolute calibration of flux measurement instrumentation for inertial confinement fusion (ICF) research. In 2009 he joined the NSLS-II project, supporting x-ray optics testing for ultrahigh resolution spectroscopy. Within NSLS-II he later took on responsibilities to lead several beamline development projects and support operating beamlines with standard detectors and other instrumentation. In 2019 Jeff took on leadership of the Engineering and Equipment (EE) group within NSLS-II's DSSI where he is responsible for defining and delivering hardware infrastructure standards supporting all beamlines at NSLS-II.

When he's not working, Jeff likes to run, make and play music, and spend time with his family.

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
2026	1993	**Dr. Jeff Keister**	*Brookhaven National Laboratory*
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 23, 2026 *(King 259)*		
10:00 am	Brian M. Getty, Lucille McGinnis, and Dr. Nathan T. Wright	Characterizing the Desmoplakin-Drug Interaction using NMR Saturation Transfer Difference Experiments
10:15 am	Logan R. Thornton and Dr. Chrisi Hughey	Use of the Opentrons Flex Automated Liquid Handling System in Teaching and Research
10:30 am	Jaimin J. Ashra, Katherine B. Weinstock, Allen C. Shepherd, James T. Whitted and Dr. Ashleigh E. Baber	Scanning for Order: Can R-2-Butanol Behave on Ni(111)
10:45 am	**Break**	
11:00 am	Katherine B. Weinstock, James T. Whitted, Allen C. Shepherd, Jaimin J. Ashra, Emily M. Euler, David W. Compton, and Dr. Ashleigh E. Baber	The Selective Catalytic Epoxidation of Ethylene on Ag/Cu(111)
11:15 am	Olivia Coer and Dr. Brycelyn Boardman	Structure-Property Relationships in Plasticized Chitosan Films: A Research Journey at JMU

Oral Session II: Thursday April 23, 2026 *(King 259)*		
1:30 pm	Elaina Manyin and Dr. Isaiah Sumner	Thermodynamics and Kinetics of Boron Esterification
1:45 pm	Rhett Sanders, Hannah Lau and Dr. Isaiah Sumner	Molecular Interactions of PET Plastic with a Lysosomal Enzyme
2:00 pm	Emily M. Euler, Haley E. Frankovich, Dr. Ashleigh E. Baber, and Dr. Kendra Letchworth-Weaver	Investigating Isomeric Butanol Reactivity and Mechanistic Pathways on TiO2/Au(111)
2:15 pm	James T. Whitted, Katherine B. Weinstock, Mollie M. Corbett, Emily M. Euler, Owen M. Paulson, Jaimin J. Ashra and Dr. Ashleigh E. Baber	Propylene Epoxidation via Ice Trapping on Cu-based Surfaces
2:30 pm	Lucille McGinnis, Brian Getty and Dr. Nathan T. Wright	Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation

(Student presenters underlined)

Poster Session: Friday April 24, 2026, 1:00 – 3:00 pm *(PCB lobby)*	
Neema Ajandeh and Dr. Barbara Reisner	Kinetic Analysis of Dye Adsorption by BNMG-1 and Granular Activated Carbon
Jacob Amberg, Deuce Irvine and Dr. Donna S. Amenta	Synthesis of N-Triazolyl and N-Pyrazolyl Derivatives as Chelating ligands for Ruthenium Complexes
Luke E. Campbell, Tyler S. Richard, Emma A. Foley, Callie R. Muska and Dr. Hui Chen	Aggregation of ultrashort-chain PFAS for target treatment via Donnan dialysis process
David W. Compton Jr, James T. Whitted, Katherine B. Weinstock, Jaimin J. Ashra, Emily M. Euler, Allen C. Shepherd and Dr. Ashleigh Baber	Unraveling the Initial Steps of Water Dissociation on Cu(111)
Brandy L. Davidson, Xeniya Kolesnikova and Dr. Gretchen M. Peters	Investigating secondary interactions in polyol-boric acid complexes in organic solvent using NMR spectroscopy
Gabriel E. Getz, Zachary D. Ryan, and Dr. Oleksandr Kokhan	3D-printed Modular Chromatography System
Kai S. Gizework and Dr. Nathan T. Wright	Understanding the Effect of Obscurin on Integrin Expression
Anna G. Grove, Conor C. Bourke, Reese E. Secord and Dr. Gretchen M. Peters	Impacts of cargo on supramolecular peptide boronic acid gels
Caitlin A. Gutierrez, Stephanie J. Schwender, and Dr. Brycelyn M. Boardman	Aggregated Induced Emission of Quinazoline Derivatives in the Presence of Glucosamine and Chitosan
Keyvan Harris, Bella Fong and Dr. Hui Chen	Sustainable Nutrient Recovery From Wastewater via Cellulose-Based Micromotors and Donnan Dialysis
Adriana Barsoom, Carly Hemani, Dr. Richard Foust and Dr. Lindsay K. Caesar	The Role of Secondary Metabolism in Heavy Metal Stress Tolerance of Subterranean Fungi
Peter Henry, Kamrin Shultz and Dr. Nathan T. Wright	Characterization of the Obscurin Functional Domain and its Regulatory Pathways
Elanor Kirkland, Kayla Moore, Dr. Brycelyn Boardman and Dr. Isaiah Sumner	Molecular Modeling Between Glucosamine and Differing Plasticizers
Colin J. Kress, Zachary H. Shelor, Donna S. Amenta, and Dr.John W. Gilje	Study of N-Benzotriazolyl Derivatives as Binding Ligands in Ruthenium Complexes
Alexander F. Lauer and Dr. J. Connor Gilhula	Creating Novel Molecular Plumbates as Potential Catalytic Anions
Daniel D Lauretti and Dr.Thomas Devore	Infrared Analysis of the Nitrate Ion with Calcium, Strontium, and Potassium
Ryan G. Marshall, Dr. Christine A. Hughey and Dr. Andrea E. Berardi	Detection of Carotenoid Pigments in Carnation Petals using UHPLC q-TOF-MS
Nathan E. Morris and Dr. Brycelyn Boardman	Understanding the Impact of Polyol Stereochemistry on Plasticized Chitosan Film Morphologies Using Scanning Electron Microscopy
Frank Muscarella, Diya Chand, Landon Gray and Dr. Lindsay Caesar	Response of Secondary Metabolism of Bat-Associated Bacteria to Chemical Stimuli
Andy A. Neumann, Alexander F. Lauer and Dr. J. Connor Gilhula	Synthesis and Metal Complexation of Regenerative Chelators for Targeted Alpha Therapy
Cameron N. Page, Dr. Gina M. MacDonald and Dr.Yanjie Zhang	Hofmeister Ion Effects on Water Structure and Caffeine Solvation
Owen M. Phillips, Dr. Thomas C. DeVore, Dr. Barbara A. Reisner, and Dr. Harry Hu	Hydrated to Anhydrous: Study of the Synthesis and Characterization of Mixed Metal Tutton Salts
Tyler S. Richard, Luke E. Campbell, and Dr. Hui Chen	Monitoring PFAS Content from Harrisonburg Drinking Water Sources via EPA Method 533
Mary M Sessoms, Mia D Fusco and Dr. Lindsay K Caesar	Discovery of Novel Metabolites from Trichoderma harzianum CO31 Isolated from a Campus Environment

Adriana Shaffner, Sarah Vollbrecht and Dr.Hui Chen	Investigating Ion Selectivity of Chelex 100 and Dowex 50W-X8 Resins for Efficient Ra^{2+} Removal From Wastewater
Max Tyree, Dr. Christine Hughey and Dr. Lillian W. Senger	Mass Spectrometric Validation of Novel Red Pigment Synthesis from Sunflower Flour
Paige O. Wooten and Dr. Gina MacDonald	Spectroscopic Studies of Environmental Influences on Protein Structure and Stability

(Student presenters underlined)

Special Announcements: Friday April 24, 2026 ***(King 159)***	
3:30pm	Announcement of Chemistry and Biochemistry Student Award Winners

Keynote Address: Friday April 24, 2026 ***(King 159)***		
3:35 - 4:35 pm	Jeff Keister, PhD JMU Class of 1993	Research: When Rubber Hits the Road

Keynote Address

Friday, April 24, 2026 at 3:35 pm
King 159

Research: When Rubber Hits the Road

Jeff Keister, PhD
(JMU Class of 1993)
Deputy Division Director, Data Science and System Integration
National Synchrotron Light Source II
Brookhaven National Laboratory
Upton, New York

Whereas university coursework prepares us with the principles of science, engaging in research forces us to take accountability for our own experimental variables. Since a predictable degree of control of conditions and accuracy in measurement are critical foundations of science, sound experimental design often leverages and expands upon established techniques, methods, and instruments. My career has largely been based on learning techniques and their engineering foundations, in order to improve their reliability and widen their applicability to scientific inquiry.

As early as during my first research at JMU, I recognized that many of the experiments I can do rely on proven instrumentation with wide applicability. Since then, I have also seen many career scientists find long-term success by developing or refining techniques which can be reliably used for many types of samples.

At the synchrotron, small beams of x-ray light with specific wavelength are delivered to a range of samples. Since the interaction of this light with samples can take an array of forms and provide correspondingly diverse types of information about the samples, scientists and engineers over time have developed many techniques which serve a wide variety of fields of study.

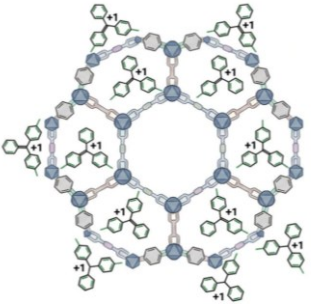
In my talk I will describe techniques I have used both in and out of the synchrotron, and I will share information about what the NSLS-II can provide to researchers in various fields as well as to students who are interested in deepening their experience with instrumentation.

STUDENT ABSTRACTS

(Student presenters underlined)

Kinetic Analysis of Dye Adsorption by BNMG-1 and Granular Activated Carbon

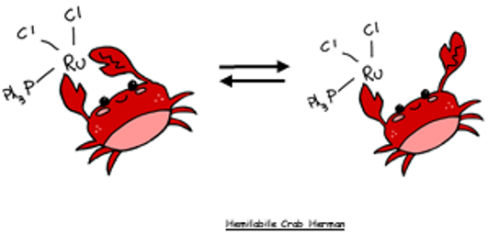
Neema Ajandeh[1] and Dr. Barbara Reisner[2]
[1]Department of Biotechnology, James Madison University, Harrisonburg, VA 22807
[2]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



BNMG-1, a copper 2-methylimidizolate metal-organic framework (MOF), is a promising adsorbent because it can be used to separate rare earth element ions from solution. It has also been suggested as a material for water remediation because it adsorbs heavy metals such as Pb(II), Ni(II), and Cd(II). In this study, the dye adsorption properties of BNMG-1 were compared to two types of granulated activated carbon (GAC). The adsorption kinetics of mono-cationic malachite green and mono-anionic bromocresol green on GAC-1079, GAC 1062, and BNMG-1 were measured using UV-VIS spectroscopy. The adsorption of these three materials, as well as the adsorption properties of GAC-1079 and GAC 1062 on other dyes, will be reported.

Synthesis of N-Triazolyl and N-Pyrazolyl Derivatives as Chelating ligands for Ruthenium Complexes

Jacob Amberg, Deuce Irvine and Dr. Donna S. Amenta
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Hemilabile Crab Mentan

Chelating hemilabile ligands are of interest for applications in organometallic catalysis. N-pyrazolyl and N-triazolyl derivatives have been studied as potential metal chelates particularly for platinum and palladium. In this study, the reaction of 1,2,3-triazole with acrylamide produced isomeric N-triazolylpropanamides L1 and L2. The synthesis of the L1/L2 mixture in dioxane was accomplished by a Michael addition in six minutes using a microwave reactor and Cs2CO3 as a catalyst. In a similar microwave reaction, the synthesis of the isomers 3-(3- methylpyrazolyl) propanamide (L3) and 3-(5-methylpyrazolyl)propanamide (L4) was accomplished in sixteen minutes. Both reactions gave good yields. When a mixture of L1 and L2 was allowed to react with n-butyllithium followed by dichlorotris(triphenylphosphine) ruthenium(II), a new phosphorus compound was obtained. The identity of the new compound is presently under investigation as is the reaction of L3 and L4 with n-butyllithium and dichlorotris(triphenylphosphine)ruthenium (II).

Scanning for Order: Can R-2-Butanol Behave on Ni(111)

Jaimin J. Ashra, Katherine B. Weinstock, Allen C. Shepherd, James T. Whitted and Dr. Ashleigh E. Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Self-assembly interactions play a vital role in natural processes such as the protein folding and micelle formation. To better understand the complexity of self-assembly, simpler model systems, such as small alcohols are often used. Previous studies have examined the self-assembly of alcohols such as R-2-butanol (R-2-BuOH) on Au(111), which forms long range, hydrogen-bonded tetramer networks. Au(111) is an inert surface with an oxophilicity of 0.0 that does not disrupt intermolecular hydrogen-bonding, allowing self-assembly interactions to dominate. To explore how surface reactivity affects self-assembly, scanning tunneling microscopy (STM) was employed to study R-2-BuOH on the more reactive Ni(111) surface. In addition to being more reactive, Ni(111) is also more oxophilic, with an oxophilicity value of 0.2. These properties result in stronger interactions between the surface and the hydroxyl group of the alcohol, which competes with intermolecular hydrogen-bonding among R-2-BuOH molecules. This competition between molecule-surface and molecule-molecule interactions interrupts long range order and inhibits self-assembly. STM imaging reveals these differences in adsorption and organization, highlighting how surface reactivity influences molecular self-assembly. Due to its higher reactivity, Ni(111) prevents extended ordering, allowing only shortrange pockets of organized structures to form.

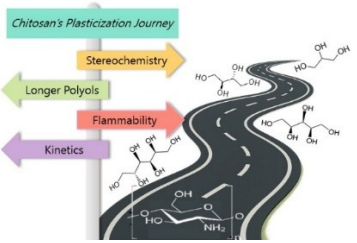
Aggregation of ultrashort-chain PFAS for target treatment via Donnan dialysis process

Luke E. Campbell, Tyler S. Richard, Emma A. Foley, Callie R. Muska and Dr. Hui Chen
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Removal of ultrashort-chain per- and polyfluoroalkyl substances (PFAS) has shown low efficiency with emerging adsorbents and ion exchange resins since they are highly mobile and less hydrophobic. Generally, with the existence of longer-chain PFAS, the adsorption of ultrashort-chain PFAS is always inhibited due to a competing effect. In this work, we employed Donnan dialysis, an ion exchange membrane process based on electrochem. potential gradients, to aggregate ultrashort-chain PFAS from a waste solution to a cleaner draw solution for further target removal. A mixture of C1-C4 PFAS solution containing 500 µg/L of trifluoroacetic acid (TFA), trifluoromethanesulfonic acid (TFMS), perfluoropropanoic acid (PFPrA), pentafluoroethanesulfonic acid (PFEtS), perfluoropropanesulfonic acid (PFPrS), perfluorobutanoic acid (PFBA) and perfluorobutanesulfonic acid (PFBS) were prepared as waste solution, and 1 M NaCl solution was put in the draw chamber. Anion exchange membranes FAA-3-PK-130 (IEC = 1.30 ± 0.15 meq/g) and FAD-PET-75 (IEC = 1.40 ± 0.10 meq/g) were investigated in this process. It is observed that the kinetics of all PFAS removal from waste solution are rapid, confirmed by pseudo first-order mechanism. On the draw side, interestingly, the aggregation rate of PFAS decreases when chain length increases, which can be attributed to the increasing hydrophobicity and higher selectivity of the longer-chain PFAS. Therefore, ultrashort-chain PFAS diffuses quickly through the membrane while longer-chain PFAS was stuck in the membrane, allowing ultrashort-chain PFAS to be efficiently treated with selective adsorbents in our future work. Overall, this work highlighted, for the first time, selective aggregation of ultrashort-chain PFAS via ion exchange membranes for target treatment.

Structure-Property Relationships in Plasticized Chitosan Films: A Research Journey at JMU

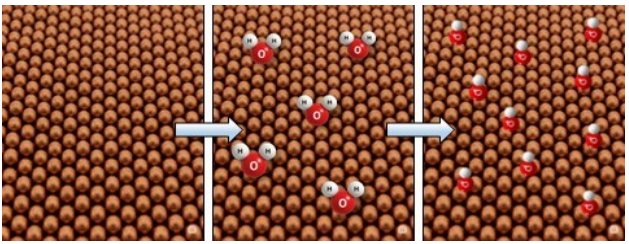
Olivia Coer and Dr. Brycelyn Boardman
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Chitosan, a natural biopolymer, is a promising alternative to petroleum-based plastics, as it combines antimicrobial and antifungal properties with natural biodegradability. Polyols and neutral polyol-boric acid (BA) complexes are commonly used as plasticizers to modify chitosan properties. However, the effects of polyol stereochemistry and chain length on these systems are not well understood. During my time in the laboratory, I have studied several polyol and polyol-BA systems with increasing complexity. This talk highlights the overarching results of this three-year study, including mechanical and thermal characterization alongside kinetic analysis of these chitosan materials.

Unraveling the Initial Steps of Water Dissociation on Cu(111)

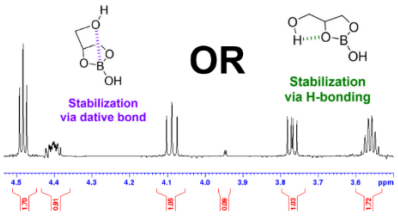
David W. Compton Jr, James T. Whitted, Katherine B. Weinstock, Jaimin J. Ashra, Emily M. Euler, Allen C. Shepherd and Dr. Ashleigh Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Copper is used in a wide range of catalytic applications, such as selective epoxidation, but results in overoxidation of reactants to combustion. Cu catalysts often depend on promoters, including Cl, Na, and Cs to reduce CO_2 emissions and enhance selectivity. However, these promoters pose environmental risks. Alternative materials have been explored to improve catalytic performance without relying on environmentally harmful promoters. The addition of Ag to Cu catalysts boosts epoxidation without the use of promoters. While Ag(111) is highly selective for epoxidation, it has a high barrier for O_2 dissociation. Cu, on the other hand, easily oxidizes. The reactive oxygen species for epoxidation are not well understood on AgCu catalysts. Exploring atomic oxygen and hydroxyl species for epoxidation will uncover the reactive oxygen necessary for selective reactions on AgCu.To systematically investigate the adsorbed atomic oxygen and hydroxyl species on model catalysts, experiments were conducted first on a Cu(111)
surface. Cu(111) readily dissociates O_2, forming atomic O on the surface, yet due to a high energy barrier, Cu(111) cannot easily dissociate H_2O. Water desorbs molecularly from Cu(111) with zero-order kinetics and a Tdes = 145-157 K. Molecular oxygen can be dosed at room temperature to promote H_2O dissociation on O/Cu(111), forming a hydroxylated surface. Temperature-programmed desorption (TPD) experiments under ultra-high vacuum (UHV) conditions show that atomic oxygen increases the desorption temperature of water by 12-15 K, stabilizing OH on the surface. The higher desorption temperature results from hydroxyl groups on the surface undergoing disproportionation. These results suggest that the stabilization of hydroxyl on the O/Cu(111) surface makes it a viable reactive oxygen species for the study of epoxidation on model catalysts.

Investigating secondary interactions in polyol-boric acid complexes in organic solvent using NMR spectroscopy

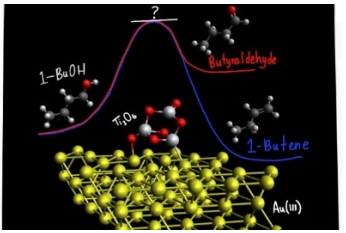
Brandy L. Davidson, Xeniya Kolesnikova and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Boric acid (BA) readily forms reversible, covalent B-O bonds with polyols, yielding complexes with broad implications for drug delivery, materials science, and polymer chemistry. While this chemistry is well-established in aqueous environments, less is known about the formation of neutral boron complexes with BA in organic solvents. Our previous work has shown that the diol binding face impacts both the product distribution and rate of this reaction, with 1,2-diols forming fastest and 1,3-diols being thermodynamically preferred. Here, we describe an NMR spectroscopic study into the complexation of polyols combined with BA. We have employed 2D NMR techniques (i.e., COSY, HSQC, and HSQC-TOCSY) to identify and fully characterize the B-O complexes formed with BA and glycerol (Glyc). Notably, the major complexes formed with these polyols are not always consistent with the trends established with diols. For example, though we would anticipate that the 1,3-isomer would predominate, Glyc forms a ~50:50 mixture of the 1,2-Glyc-BA and 1,3-Glyc-BA complex when BA is added. We theorize that this is due to stabilizing interactions between the free OH of the polyol and the B-O ring. Support for this hypothesis has been seen computationally and via spectroscopic methods with triols of longer tail length, such as 1,2,4-butanetriol (1,2,4-BT), 1,2,5-pentanetriol (1,2,5-PT), 1,2,6-hexanetriol (1,2,6-HT), and 1,2,10-decanetriol (1,2,10-DT). The impact of the linker length, as well as additional stabilization from intramolecular interactions were investigated. In combination, these findings highlight the impact of structural features within the polyol on the formation of B-O complexes. In the future, we will use these results as a scaffold for solving more complex structures and will evaluate the thermodynamics and kinetics of polyol-BA complexation.

Investigating Isomeric Butanol Reactivity and Mechanistic Pathways on TiO2/Au(111)

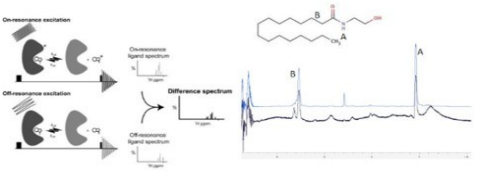
Emily M. Euler, Haley E. Frankovich, Dr. Ashleigh E. Baber, and Dr. Kendra Letchworth-Weaver
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



A promising route for fossil-fuel-free plastic production involves the selective dehydration of biomass-sourced small alcohols to alkenes over heterogeneous model catalysts. For instance, the selective dehydration of biobutanol (butanol sourced from biomass) can enable the formation of the valuable plastic precursor, butene. Developing a deeper understanding of the fundamental thermal catalytic processes of butanol over heterogeneous model catalysts aids in the design of more efficient catalysts. Temperature-programmed desorption (TPD) experiments demonstrate differences in both reactivity and selectivity for butanol isomers. 1-BuOH reveals little reactivity and high selectivity for butene (reduced) products, whereas 2-BuOH displays high reactivity and low selectivity, producing both 2-butanone (oxidized) and butene (reduced) products. To gain an atomically-detailed perspective on these processes, density functional theory (DFT) was used to investigate energetic trends and identify comparisons between 1- and 2-BuOH as they adsorb on Ti3Ox nanoparticles supported on a Au(111) surface. Findings suggest Ti-OBuOH bonding, van der Waals interactions between the alkane chain and the Au surface, and electrostatic interactions between H and the nanoparticle all impact butanol's interactions on the catalyst material. Adsorption energies of both BuOH isomers place greater significance on Au surface interactions over Ti coordination number in determining favorability. Calculated bond distances suggest that the configuration of 2-BuOH enables it to interact more favorably with both the nanoparticle and Au surface compared to 1-BuOH, leading to greater reactivity. Transition state energetics support experimentally observed trends for the thermodynamic favorability of 2-BuOH forming oxidized products compared to 1-BuOH.

Characterizing the Desmoplakin-Drug Interaction using NMR Saturation Transfer Difference Experiments

Brian M. Getty, Lucille McGinnis, 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. However, parameters of how these drugs interact with DSP, including binding affinity, the binding orientation, and bioavailability in our system, are unknown. Here, using NMR saturation transfer difference (STD) experiments, we begin to quantify these characteristics of each DSP degradation-inhibiting small molecule in the presence of wild-type (WT) and mutant DSP strands. Future work will continue identifying these characteristics for each small molecule and calpain-sensitive mutation strain.

3D-printed Modular Chromatography System

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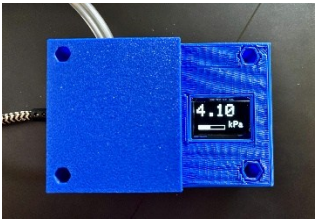

Liquid chromatography (LC) systems are prohibitively expensive for undergraduate education and research. To more broadly introduce liquid chromatography to education and research, we are developing a modular, open-source chromatography system. This work describes our progress in developing an LC system designed for biochemistry teaching labs and aimed at faculty interested in introducing analytical instrumentation activities in the curriculum. Fluid flow is provided by a 3D-printed peristaltic pump utilizing common hobbyist robotics motors, 3D-printing stepper motors, and motor driver circuits. A pressure sensor board with an LCD display and 3D-printed housing has been designed to integrate into this system with a 3D-printed T-junction connector. As pressure increases in the system, a progress bar displays the maximum safe pressure, and if this threshold is crossed, a loud beep will notify students to reduce the flow rate. This allows for safe and efficient pump usage. The development of a conductivity sensor and a fraction collector is also underway. Weak signals from various detectors are amplified using a modular amplifier, capable of amplifying up to 2 signals at once. In this chapter, we describe our progress towards the development of a UV detector composed of a 3D-printed flow cell with glass coverslip windows, a UV LED, and a UV photodiode that does not require focusing lenses. We specifically focus on several open-ended activities that enable students to optimize detector performance for specific experimental needs and to introduce key concepts of analytical instrumentation. 3D models are developed online through Tinkercad and illustrate the role of 3D-printing in enabling instrumentation projects. All 3D printing files, electronic schematics, and Gerber files are available on GitHub with a GNU 3.0 license. Ultimately, we aim to introduce this work into undergraduate teaching and research labs, while this chapter prioritizes educational instrumentation activities enabled by 3D printing.

Understanding the Effect of Obscurin on Integrin Expression

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Obscurin is a large modular cytoskeletal protein which holds the ability to influence cell motility and migration, including membrane and cytoskeletal organization. Obscurin knockout results in increased migration and begins the epithelial-to-mesenchymal transition. Clinically, obscurin is the second most mutated protein found in breast and colorectal cancers along with significant downregulation in pancreatic cancers. Among the downstream obscurin targets are cell adhesion molecules such as integrin and cadherin. These proteins regulate the extent to which cells adhere to each other and to the basal lamina and are thus intrinsically linked to cell motility. Here, we explore whether obscurin alters integrin b3 expression through western blot analysis of obscurin-infected MDCK cells. We find that obscurin upregulates integrin expression, and further that multiple signalling domains in obscurin are redundantly responsible for this upregulation. These studies agree with previous work in our lab showing that obscurin acts through both a RhoA-dependent and a PI3K-dependent pathway to modulate cell motility.

Impacts of cargo on supramolecular peptide boronic acid gels

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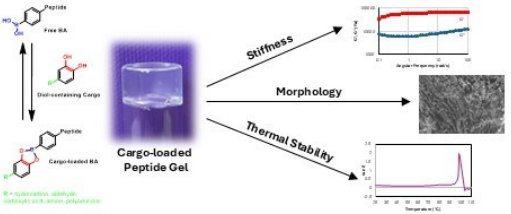

Supramolecular gels have been widely used for cargo-loading applications, including drug delivery and environmental clean-up. Peptide gelators are particularly attractive for this function, as they generally have high biocompatibility, low critical gelation concentrations (CGC), and are stimuli-responsive. Generally, the incorporation of target molecules into peptide gels has utilized diffusion mechanisms or hydrophobic forces, which lack specificity and are difficult to control. Here, we report a supramolecular peptide hydrogel capable of selectively binding to diol-rich cargo via reversible boronate ester bonds. Triphenylalanine boronic acid ([Phe]3BA) was found to form stiff, stable hydrogels at concentrations greater than 2 mM at neutral pH. Spectroscopic studies indicate that [Phe]3BA forms β-sheets and that the B(OH)2 group is free and accessible for binding. A variety of catechol derivatives, an important class of compounds commonly used in pharmaceuticals, pesticides, and dyes, were incorporated into the [Phe]3BA gel via covalent B-O bond formation. Structurally, we observed that catechol derivatives with alkyl, amine, or aldehyde substituents were well-tolerated in the gel, having little to no impact on the rheological properties. In contrast, carboxylic acid-containing catechol derivatives notably decreased the material stiffness. We theorize that these functional groups disrupt noncovalent interactions between peptide units, thereby destabilizing the gel network. Further investigation of the gels morphology and thermal stability based on functionalized catechol derivatives indicate similar trends, but this work is in development. These results provide important insights into using boronic acid units in peptide gels for targeted cargo loading. Additionally, we have demonstrated that [Phe]3BA gels have outstanding potential as materials for cargo-based applications.

Aggregated Induced Emission of Quinazoline Derivatives in the Presence of Glucosamine and Chitosan

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Antisense 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 promote aggregation-induced emission (AIE) in HPQ turning the sensor to the “on” state. HPQ-Ac was incorporated into chitosan films, however these films fluoresced 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. 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. Additional quinazoline derivatives were prepared to investigate the impact of hydrogen bonding capability and steric bulk on the interaction of these sensor molecules with GlcN and chitosan. 2-(Phenyl)quinazolin-4(3H)-one (PQ), acetylated 2-(2-hydroxy-3,5dit-butylphenyl)quinazolin-4(3H)-one (BPQ-Ac) and 2-(2-hydroxy-3,5dit-butylphenyl)quinazolin-4(3H)-one (BPQ) were prepare under similar reaction conditions to HPQ and HPQ-Ac. Even in the absence of hydrogen bonding capabilities, PQ still displays fluorescence intensity in solution, in the presence of GlcN, in chitosan solution and films. This result suggests that hydrogen bonding interactions with the chitosan chains are not responsible for the “on” state of the fluorophore, but that the molecule is capable of pi-pi stacking that initiates the AIE. Both BPQ and BPQ-Ac have reduced fluorescence intensity in solution when compared to HPQ and PQ. Interestingly, BPQ shows an increase in fluorescence intensity in the presence of GlcN while BPQ-Ac does not. Additionally, chitosan films containing BPQ-Ac have a significantly reduced emission intensity compared to other derivatives. These films were then exposed to amine vapor and fluorescence was turned “on” These combined results indicate, that steric bulk is the most promising structural modification for use of quinazoline derivatives as sensors in chitosan films.

Sustainable Nutrient Recovery From Wastewater via Cellulose-Based Micromotors and Donnan Dialysis

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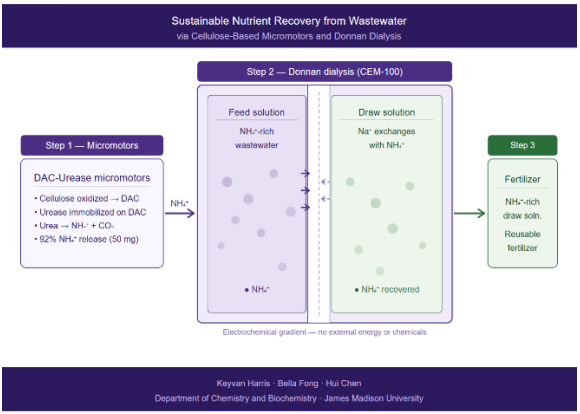

Nutrient pollution is a major environmental challenge driven largely by nitrogen- and phosphorus-rich animal manure waste. Recovering these nutrients for beneficial reuse offers a sustainable pathway to mitigate pollution while producing valuable fertilizers. In this study, we developed cellulose-based micromotors to promote nitrogen release from urea-containing wastewater and coupled the process with Donnan dialysis for ammonium recovery. The micromotors were sequentially fabricated by oxidizing cellulose to dialdehyde cellulose (DAC), followed by immobilization of urease to form DAC-urease. The immobilized urease catalyzed urea hydrolysis in model wastewater, producing NH_3 and CO_2, with NH_3 subsequently converting to soluble NH_4^+. Donnan dialysis was then employed to recover NH_4^+ into a cleaner draw solution using a CEM 100 cation exchange membrane. Driven by electrochemical potential gradients, Na^+ in the draw solution exchanged with NH_4^+ in the feed solution without external energy or chemical addition. The developed micromotors were dosed into urea-containing model wastewater, and NH_4^+ transport to the draw side was monitored to evaluate recovery performance. This integrated micromotor–Donnan dialysis approach demonstrates a sustainable strategy for nutrient recovery and fertilizer production from nitrogen-rich waste streams.

The Role of Secondary Metabolism in Heavy Metal Stress Tolerance of Subterranean Fungi

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Heavy metals pose a significant risk to public safety for all humans, animals, and living organisms in the environment. The effective detoxification and removal of metal contaminants from polluted environments have increasingly moved towards bioremediation by specialized microorganisms as a sustainable solution to mitigate the negative environmental impacts of mining. Given that caves are extreme environments containing heavy metals due to both natural and anthropogenic factors, we predicted that subterranean fungi will be privileged for heavy metal stress tolerance. Our team isolated 17 fungal strains from Grand Caverns, the country's oldest show cave, and performed preliminary growth assays across a spectrum of heavy metal concentrations using chloride salts of copper, nickel, and cadmium. The analyzed fungi yielded 4/17 (23%) tolerant samples to concentrations of cadmium and/or nickel $\geqslant$5mM. Our team is interested in observing the bioremediative potential of the Grand Caverns fungi as well as the role of secondary metabolism in their heavy metal stress tolerance. Tolerant fungi underwent three heavy metal tolerance screens with increasing concentrations of heavy metal salts to ascertain the maximum concentration of heavy metals each fungi can endure, following which heavy metal bioaccumulation will be quantified using ICP-OES to evaluate the bioremediative potential of fungi from Grand Caverns. To evaluate the role of secondary metabolism, tolerant fungi were also subjected to comparative growth assays to identify molecules that were associated with metal-containing conditions. Preliminary mass spectrometry analysis of metal-tolerant Leptobacillium leptobactrum CH-001 revealed upregulation of several oxopyrrolidine derivatives in the presence of cadmium. As oxopyrrolidine-based ligands display metal-chelating properties and have been utilized as anticancer metallodrugs, these results suggest that subterranean fungi take advantage of biomedically relevant metallophores to achieve heavy metal tolerance. Continuing studies are underway to evaluate the capabilities of additional fungal strains.

Characterization of the Obscurin Functional Domain and its Regulatory Pathways

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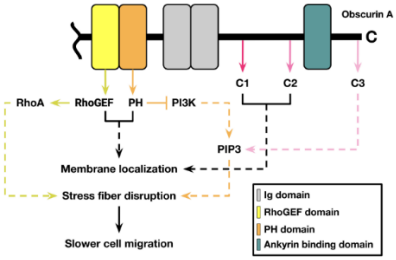

The cytoskeletal protein obscurin has previously been studied only in muscular cells, where it was first characterized. It is known that obscurin plays a role in cell mobility, and if not functioning correctly, can lead to cancer as a result of unregulated movement. Literature has shown that this protein is most often mutated in breast and colorectal cancers. In novel experiments, obscurin is added to cell cultures via adenovirus infection as opposed to previous methods utilizing knockout techniques. The effects of this addition have been measured in colocalization studies, timelapse velocity analysis, and lipid assays. Each of these experiments has shown that there are multiple domains within the obscurin construct that oversee cellular mobility regulation, namely the Rho-GEF and PH domains, as well as certain segments of the unstructured region near the C-terminus of the protein.

Molecular Modeling Between Glucosamine and Differing Plasticizers

Elanor Kirkland, Kayla Moore, Dr. Brycelyn Boardman and Dr. Isaiah Sumner
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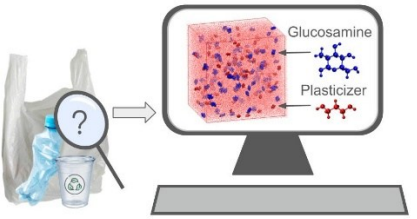

Bioplastics are an environmentally friendly alternative to traditional petroleum based synthetic polymers. Chitosan based bioplastics have emerged as a promising alternative due to their biodegradability and renewable sources. Made from two main parts, chitosan – an abundant biopolymer derived from chitin found in the exoskeleton of arthropods – and a plasticizer – an additive that can change the physical properties of chitosan. Despite their potential, the molecular-level interactions between chitosan and plasticizers, and how these interactions influence macroscopic behavior, remain poorly understood. Computational modeling provides a powerful approach for developing rational design strategies by enabling the prediction of polymer behavior. To address this, we previously modeled interactions between β-D-glucosamine and several polyol plasticizers. Quantum calculations identified stable structures and suggested that diols promote glucosamine aggregation. IR modeling of amine blue shifts showed mixed agreement, indicating additional environmental and competing effects. To further advance this research, molecular dynamics simulations are being explored to investigate the dynamic behavior of the interactions between chitosan and plasticizers. Several different ratios of glucosamine and glycerol (50:50, 50:25, and 75:25) in a solution of water and acetic acid provide deeper insight into how these components interact in a larger, more complex system. Simulating more realistic conditions reveals valuable insights into the structural stability, molecular aggregation, and overall compatibility of chitosan based bioplastics.

Study of N-Benzotriazolyl Derivatives as Binding Ligands in Ruthenium Complexes

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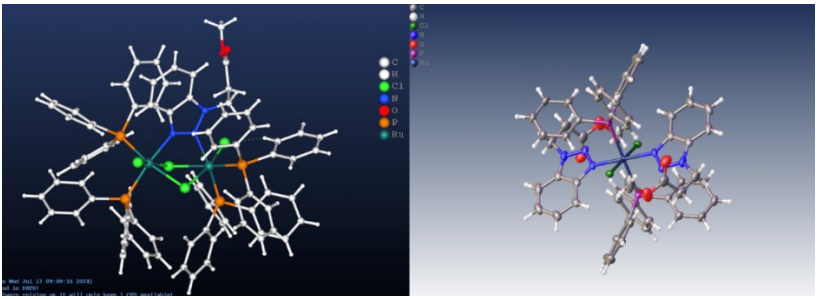

In this study, we investigate the asymmetric ligand N-benzotriazolylpropanoate (L1) as a potential hemilabile ligand capable of coordinating to metal centers through either a heterocyclic nitrogen donor or an oxygen donor from the carboxylate moiety. The ligand was synthesized via a solvent-free, catalyst-free Michael addition of benzotriazole with methylacrylate, yielding two ester products, L1 and L2. After separation of L1 and L2, the study of the coordination chemistry of L1 with dichlorotris (triphenylphosphine) ruthenium(II), $RuCl_2(PPh_3)_3$, was explored. To better understand this behavior, a systematic investigation of differing ligand-to-metal ratios was conducted, demonstrating that variations in stoichiometry significantly influence product distribution and coordination environments. Analysis by ^{31}P NMR spectroscopy of the product isolated from reaction solutions in CD_2Cl_2 revealed the formation of multiple products, suggesting complex speciation in solution. These species have not yet been fully resolved or individually characterized. When the reaction of L1 and $RuCl_2(PPh_3)_3$ (2:1 ratio) is performed in acetone and minor volume of toluene (23mL/2mL) to help increase the solubility of $RuCl_2(PPh_3)_3$. After four weeks, red/orange crystals precipitate from the reaction mixture. These crystals were characterized by ^{31}P NMR and infrared spectroscopy, elemental analysis, and single-crystal X-ray diffraction, confirming its coordination mode and structural features. Similarly, a 1:2 ratio of ligand to $RuCl_2(PPh_3)_3$ in the acetone/toluene solvent system yielded a red precipitate after 10 minutes, for which a partially refined single crystal structure was obtained. Time-dependent rearrangement of the 2:1 and 1:2 products in CD_2Cl_2 have been observed in the ^{31}P NMR spectra. Ongoing studies are focused on these time and solvent dependent rearrangements, providing further insight into the dynamic behavior and hemilabile nature of the complex.

Creating Novel Molecular Plumbates as Potential Catalytic Anions

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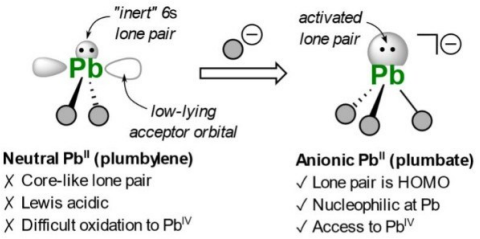

Lead (Pb), as one of the most abundant elements in the Earth's crust, is well poised to overcome economic and sustainability concerns presented by precious metal shortages caused by current geopolitical tensions. A key challenge which has so far stunted Pb as a catalytic element is its strong resistance to 2-electron redox cycling. We hypothesize that molecular plumbates—tricoordinate, anionic species that are known to react as Pb nucleophiles—have potential to engage in catalytic redox cycling which mimics platinum and palladium reactivity. This work explots the strong chemical analogy between Pd and Pb which has been known for nearly fifty years. These plumbates would present a more cost-effective and sustainable catalyst for the formation of carbon–carbon bonds than current precious metals. We have taken on the challenge of "resurrecting" these under-investigated compounds by expanding the scope of known plumbates in a synthetic chemistry campaign. We found that homoleptic trithiolatoplumbates [Pb(SR3)–] are formed by treating polymeric, insoluble Pb(SR)2 with a suitable thiolate salt in methanol. We have also successfully accessed trihaloplumbates (PbX3–; X = Cl, Br). We have identified these compounds unambiguously by 207Pb NMR spectroscopy, which is a new analytical capability that we have established for JMU. We envision that these preliminary studies will represent a first step towards establishing a catalytic cycle that enables precious element-like reactivity at a Pb center.

Infrared Analysis of the Nitrate Ion with Calcium, Strontium, and Potassium

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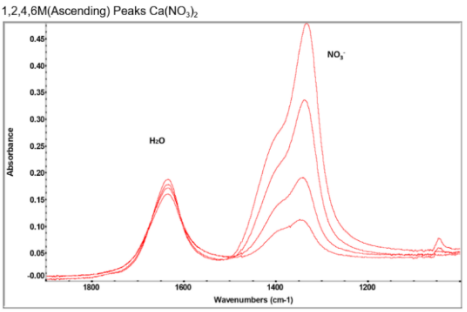

Since most inorganic nitrates are water soluble, the nitrate ion is a wide-spread ground water contaminant. Nitrate exposure above the 10 mg/L limit for drinking water set by the EPA has been linked to cancer and thyroid disease. Attenuated total reflectance -Fourier transform infrared spectroscopy (ATR-FTIR) is a rapid, non-destructive way to test for nitrate in water. While the well-known Lewis dot structure for nitrate (NO3-) indicates it is planar with D3h symmetry and should have only 1 IR active asymmetric stretch, the broad IR band in the asymmetric N-O stretching region at approximately 1400 cm-1 has long been known to split into two bands. We are investigating the ATR-FTIR spectra for a concentration series of potassium, calcium and strontium nitrates to attempt to gain a better understanding about the interactions occurring in aqueous nitrate solutions.

Thermodynamics and Kinetics of Boron Esterification

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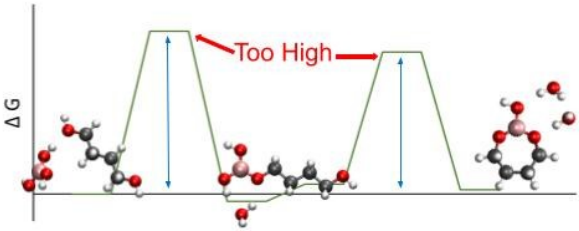

Biodegradable plastics are alternatives to current plastics as they are more environmentally friendly. Bioplastics made from chitosan can be tuned using plasticizers. In recent experiments, borate esters with glycerol were used as plasticizers for the polymer. Although this combination resulted in poor plasticity, borate ester plastics present desirable properties, such as stiffness and thermal stability, that warrant more investigation. However, the molecular-level understanding of borate ester synthesis is unexplored. Borate esters synthesized from boric acid and diols can form open-chain or cyclic complexes. Experimentally, reactions with ethane glycol and 1,3-propanediol formed mostly closed cyclic complexes, whereas reactions with 1,4-butanediol formed only open-chain complexes. To explain experimental data, Gibb's free energies were calculated using density functional theory (DFT) at the M06-2x/6-311+G(2d,p) level-of-theory. ΔG values were calculated by subtracting the closed complex plus a free water molecule needed to balance the reaction by the open complex (ΔG= (Gclosed+GH2O) – Gopen). Ethane Glycol Boric Acid, 1,3-Propanediol Boric Acid, and 1,4-Butanediol Boric Acid produced ΔG values of -1.45 kcal/mol, -6.86 kcal/mol, and -0.69 kcal/mol, respectively. Although computational findings did not match experimental data, the trend of how favored the closed complex was in each diol boric acid did. To explain these observations, the reaction barrier heights were explored to investigate the kinetics of formation of these reactions. In all proposed mechanisms two transition states and two different intermediates to form the product for each reaction were found. However, the barrier heights were unrealistically high in energy suggesting a more complicated reaction mechanism forms these complexes. To address this, the Synchronous Transit-guided Quasi-Newton (QST2) method was conducted to locate transition states. New transition states were found for each diol boric acid, yet the same barrier height challenges were produced.

Detection of Carotenoid Pigments in Carnation Petals using UHPLC q-TOF-MS

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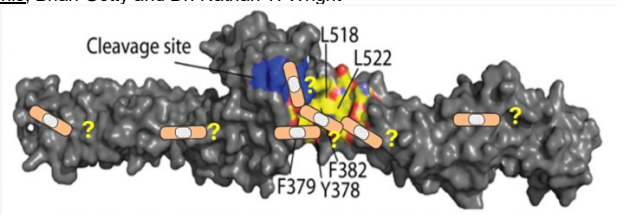
Pigmentation in flowering plants is primarily driven by anthocyanins and carotenoids, yet the relative contributions of these pigment classes remain unresolved in many Caryophyllaceae taxa. Within the genus Silene, red floral coloration is rare, phylogenetically restricted, and frequently associated with polyploid lineages, suggesting a biochemical basis that requires comprehensive metabolomic characterization. While core pigment biosynthetic pathways are broadly conserved, structural diversity arises from modification of pigment backbones through varied substituents, motivating detailed chemical profiling. This study establishes an end-to-end analytical workflow for carotenoid extraction and characterization from petal tissue to support ongoing investigations of pigment composition in Caryophyllaceae, where anthocyanins are relatively well characterized in Silene but carotenoids remain poorly defined. Dianthus caryophyllus (carnation) petals were studied as a model system for method development due to their phylogenetic similarity to Silene and the existence of well-documented carotenoid profiles, providing a validated benchmark for later application to less-characterized taxa. Petal tissue from a yellow cultivar was cryogenically homogenized and extracted using acetone buffered with Tris-HCl. Pigments were partitioned into diethyl ether via sequential liquid-liquid extraction, followed by aqueous washing to improve phase selectivity. The organic phase was evaporated under nitrogen, reconstituted in methanol, and analyzed by ultra-high-performance liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (UHPLC–QTOF-MS). Preliminary datasets reveal thousands of detected features, reflecting substantial chemical complexity and co-extraction of non-carotenoid metabolites (e.g. lipids). Despite this, target carotenoids (lutein, β-carotene, β-cryptoxanthin, zeaxanthin, antheraxanthin, violaxanthin, and neoxanthin) were successfully annotated. Ongoing work will apply chemometric approaches to improve discrimination of carotenoids from co-extracted compounds, while tandem mass spectrometry (MS/MS) will be used to confirm identities of analytes lacking authentic standards. This workflow establishes a robust analytical pipeline from tissue preparation to carotenoid profiling and provides a foundation for understanding the biochemical mechanisms underlying red floral coloration in Silene.

Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation

Lucille McGinnis, Brian Getty and Dr. Nathan T. Wright



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 μM range. Here we begin studies designed to interrogate where the most promising drugs bind to desmoplakin, using molecular dynamics experiments.

Understanding the Impact of Polyol Stereochemistry on Plasticized Chitosan Film Morphologies Using Scanning Electron Microscopy

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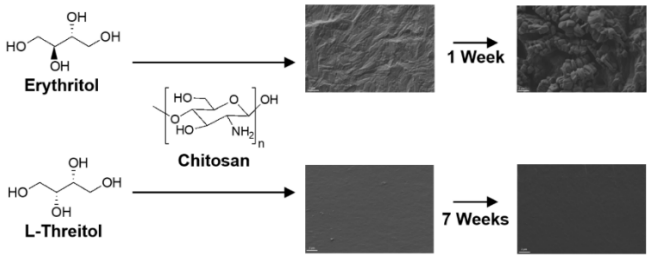

Correlating physical and mechanical properties to surface morphologies can be very challenging in complex polymer systems whereas cross-sectional images are much more valuable. Herein we describe the investigation of both surface and cross-sectional morphologies of chitosan films plasticized with the stereoisomers L-threitol (L-Thr), and erythritol (Ery) in the presence and absence of boric acid (BA). Our previous results have shown that the addition of glycerol reduces the pore-like structures observed in pure chitosan films, and the addition of BA to the system yields a more uniform morphology with a reduction of pore size. SEM images were collected overtime on the same chitosan film samples which contained increasing amounts of the polyols (25 mM-100mM). Visible aging of the films from transparent to opaque was correlated to the increasing presence of microstructures on the surface and cross-section of the films in the SEM images. L-Thr films displayed significantly different rates of microstructure formation comparted to Ery, indicating that stereochemistry does play a role in the interaction of the polyol with the chitosan chains and the migration of the polyol through the polymeric network. Similar experiments were performed with films containing chitosan, polyols (25 mM-100mM) and the addition of BA (0.5 eq-2.0 eq). SEM images indicate that as BA equivalents are increased, the aging process is inhibited, with little to no microstructure formation observed, even at extended time points. Differences in the pore-sizes were also observed when compared to previously studied Glycerol-BA films. Both L-Thr-BA and Ery-BA containing films showed a significant reduction in pore-size and an increase in the smoothness of the cross-sections. Additional films containing stereoisomers sorbitol and mannitol also revealed significantly different cross-sectional morphologies, further supporting that the stereochemistry of the polyol does impact the interactions between the plasticizer and the chitosan chains even in extended polyol systems. This study continues to aid in our development of a methodology for tuning and optimizing chitosan materials.

Response of Secondary Metabolism of Bat-Associated Bacteria to Chemical Stimuli

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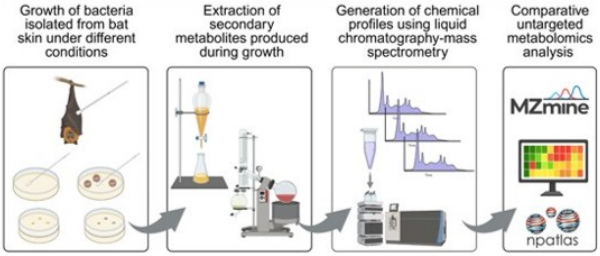
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



Bat populations in North America are in decline due to Pseudogymnoascus destructans, the fungus that causes White-Nose Syndrome (WNS). Despite the spread of WNS across the United States, many bats remain WNS-free, potentially due to the protective effect of their skin microbiome. To evaluate the antifungal potential of bat-associated bacteria, 632 bacteria from WNS-free bats in New Mexico were isolated, 36 of which inhibited P. destructans. The molecules responsible for this antifungal activity were not explored. Unfortunately, most natural product biosynthetic pathways are turned off under laboratory conditions, making it difficult to evaluate the antifungal potential of organisms in a laboratory setting. To overcome the limitations of traditional culturing methods, we used the “One Strain Many Compounds” (OSMAC) approach, in which culture conditions are altered to activate silent biosynthetic pathways. To maximally express natural products, in twelve strains of bat-associated bacteria were grown under standard conditions, with the histone deacetylase inhibitor suberoylanilide hydroxamic acid (SAHA), or with lanthanum (III) chloride. Chemical changes were evaluated using mass spectrometry. Using publicly available natural products databases, we have putatively identified 21 molecules that are reproducibly upregulated in SAHA- or lanthanum-treated cultures. Current studies evaluating the impact of scandium (III) chloride and N-acetylglucosamine on natural product production are underway.

Synthesis and Metal Complexation of Regenerative Chelators for Targeted Alpha Therapy

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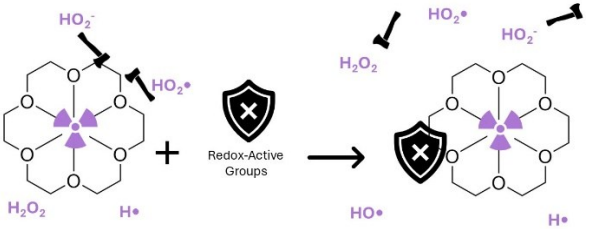

New advances in radiotherapy are moving further down the periodic table in search of innovative approaches to cancer treatments. Targeted alpha therapy is one such method that uses high energy alpha particles from the radioactive decay of chelated (i.e., complexed) atoms to attack cancerous tissue, leaving neighboring cells largely unharmed. However, few chelators in aqueous environments can withstand the effects of ionizing radiation without breaking apart and releasing their radioactive isotope due to the creation of reactive oxygen species (ROS). To address this problem, we have made progress toward novel dibenzo-18-crown-6 derivatives that utilize redox-cyclable anthraquinone groups to catalytically neutralize ROS. Initial experiments were successful in rapidly binding non-radioactive surrogates La3+, Ba2+, and Sr2+ to a simplified phosphonate-substituted and pentaethylene glycol macrocycles. We established a new radioanalytical capability (radio-TLC) at JMU to demonstrate that ions of uranium-238 are also bound by this crown ether derivative. Future work in the project will consist of completing our proposed synthesis of redox-active complexing agents, evaluating their stability under radiolytic conditions at Madison Accelerator Laboratory, and binding clinically suitable isotopes like radium-223 and actinium-225 to these self-regenerative chelators.

Hofmeister Ion Effects on Water Structure and Caffeine Solvation

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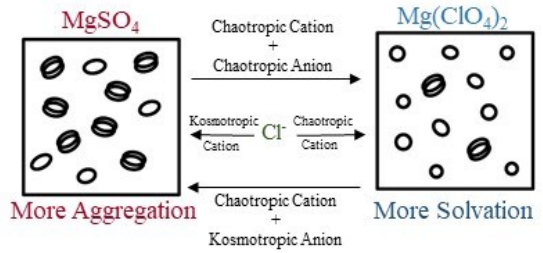

The Hofmeister series is a list of ions ranked on their ability to salt in or salt out proteins. Caffeine was used a as model compound to investigate how different combinations of various kosmotropic and chaotropic ions influence caffeine solvation and aggregation. Anionic effects on caffeine have been previously studied in depth, however fewer studies have been performed using cations. Previous studies have shown that the presence of Hofmeister ions alters water structure. Kosmotropic ions increase hydrogen bonding and chaotropic ions decrease water hydrogen bonding. Attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) was utilized to study the relative solvation of the caffeine molecules in various salt solutions. Our results demonstrate that a chaotropic cation with a chaotropic anion (Mg(ClO4)2), leads to a decrease of the two caffeine carbonyl stretching vibrations at ~1698 cm-1 and ~1638 cm-1, indicating increased caffeine solvation. However, a chaotropic cation with a kosmotropic anion (MgSO4), leads to increases of the two carbonyl peaks, indicating increased caffeine aggregation. Our results suggest for most ion combinations that the anionic effects dominated the cationic effects, with the exception of the chloride anion. Interestingly for the chloride anion, our results showed that the cationic effects dominated. Kosmotropic cations (NH4+, Na+) increasing caffeine aggregation and chaotropic cations (K+ , Mg2+) increasing caffeine solvation. The anionic effects mostly dominated the water structure, with some exceptions.

Hydrated to Anhydrous: Study of the Synthesis and Characterization of Mixed Metal Tutton Salts

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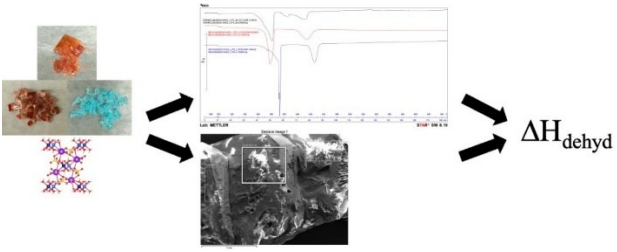

Tutton salts are a family of double salts with applications in waste heat recovery and solar energy storage. In this study, mixed-metal Tutton salts with the formula K2CuxCoyZnz(SO4)2·6H2O, K2CuxZnz(SO4)2·6H2O, K2CoyZnz(SO4)2·6H2O, and K2CuxCoy(SO4)2·6H2O were synthesized by slow evaporation. The synthesized salts were then analyzed and characterized using as Powder X-ray Diffraction (PXRD), Infrared Spectroscopy (IR), Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS), and Differential Scanning Calorimetry (DSC). SEM/EDS was used to determine the average chemical formula for each of the salts. DSC analysis gave a range for dehydration enthalpies from 323.44-347.08 kJ/mol for the salt series. Aside from initial characterization of the salt, PXRD and IR were used to determine the change in the structure of the K2CuxCoy(SO4)2·6H2O salt as it was heated to different temperatures. It was found that when heating the salt becomes amorphous to x-rays before becoming crystalline again at higher temperatures. Additionally, the dehydrated salts were able to be rehydrated indicating that the salts could be used in thermal storage situations.

Monitoring PFAS Content from Harrisonburg Drinking Water Sources via EPA Method 533

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Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants of emerging concern in drinking water sources due to their environmental persistence and potential health risks. This project investigated PFAS occurrence in the Shenandoah River, a drinking water source for Harrisonburg, Virginia, through a collaborative effort with the Department of Engineering and Harrisonburg Public Works. Water samples were collected weekly and analyzed using EPA Method 533 to monitor PFAS occurrence and temporal variation. Sample preparation involved solid-phase extraction (SPE) to concentrate target analytes while removing salts and other matrix interferences. The extracted samples were then reconstituted in an ethanol-based solution prior to liquid chromatography–mass spectrometry (LC/MS) analysis. A suite of more than 24 PFAS compounds was targeted for quantification. Weekly monitoring enabled evaluation of PFAS presence, concentration variability, and potential trends over time. This study provides critical baseline data for PFAS occurrence in a regional drinking water source and supports ongoing assessment of PFAS contamination and risk management strategies.

Discovery of Novel Metabolites from Trichoderma harzianum CO31 Isolated from a Campus Environment

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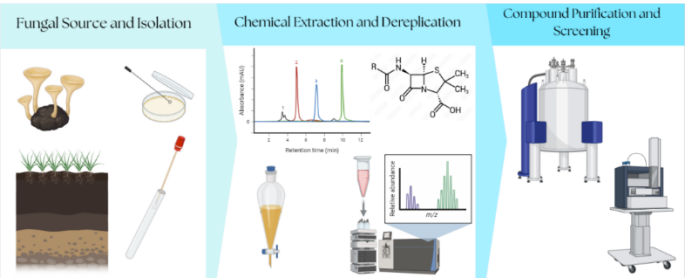

Natural products research has historically led to the discovery of transformative therapeutics, including antibiotics, antifungals, anticancer agents, and immunosuppressants. These studies remain essential because natural sources provide structurally diverse and biologically active compounds that continue to inspire new drug leads and biochemical tools. Among these sources, fungi are particularly valuable due to their high metabolic diversity and ability to produce unique secondary metabolites with a wide range of biological activities. Unlocking this chemical potential requires systematic workflows for the collection, cultivation, extraction, purification, and dereplication of fungal metabolites. To harness these compounds, fungal isolates undergo a series of inoculation, fermentation, and regrowth steps designed to optimize metabolite production. Dereplication is an essential early step in natural products discovery, and it allows for the identification of known compounds and avoids rediscovery, focusing efforts on potentially new chemical entities. Prioritized extracts are then subjected to chromatographic separation and high-resolution analytical techniques, such as liquid chromatography and mass spectrometry. In this lab, dereplication data were compared against a database at UNC Greensboro to match sample characteristics and IDs with previously characterized metabolites, as well as the public database, NPAtlas. Chemical data from one fungal strain, Trichoderma harzianum C031, isolated from JMU's campus, indicated that the fungus produced twelve prominent metabolites that did not match existing molecules in the natural products databases, indicating the presence of potentially new chemical entities. Since this discovery, T. harzianum C031 has been grown in bulk culture and subjected to flash chromatography to purify the potentially novel molecules and elucidate their structures using NMR spectroscopy. This approach supports the identification of unique natural products and aids the overall goal of discovering new bioactive compounds from fungal sources by focusing on the most promising candidates.

Molecular Interactions of PET Plastic with a Lysosomal Enzyme

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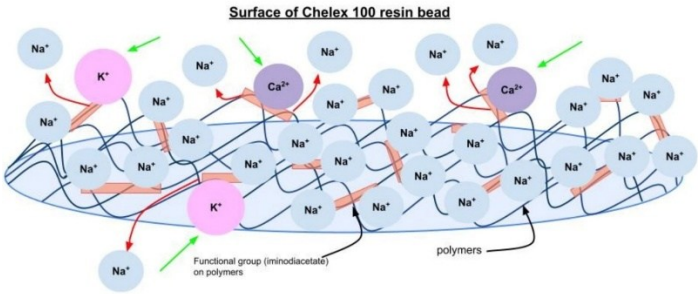
Plastics continuously decompose into tiny, tiny pieces called microplastics which are absorbed into our bodies by oral intake, inhalation, and skin contact. They then travel into our bloodstream and interact with organelles and proteins in our cells, which may cause damage and lead to disease. Unfortunately, we currently do not have a detailed understanding of how microplastics interfere with our biochemistry, although some details are emerging. For example, there is evidence that polyethylene terephthalate (PET), a common plastic which makes up much of the food and beverage packaging, slows down the lysosome, an organelle that disposes of cellular waste, but there is currently no molecular-level understanding of this process. We hypothesize that PET may inhibit the normal function of lysosomal enzymes that digest molecules with structures similar to PET. To test this hypothesis, we focused our efforts on interactions between PET and Lysosomal Acid Lipase (LAL), an enzyme that cleaves large fatty substrates into small nutrients. We are investigating this interaction through docking software (AutoDock Vina and Diffdock), molecular dynamics simulations (AMBER), and binding energy calculations. First, the PET was placed into LAL's binding pocket with docking software. Second, molecular dynamics simulations were used to see if the PET would remain bound to the active site and to quantify active-site interactions. Finally, binding energy calculations were initiated. Our simulations show that it is likely that PET does bind to LAL's active site.

Investigating Ion Selectivity of Chelex 100 and Dowex 50W-X8 Resins for Efficient Ra^{2+} Removal From Wastewater

Adriana Shaffner, Sarah Vollbrecht and Dr.Hui Chen
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



This project investigated the ion selectivity of two cation exchange resins: Dowex 50W-X8 (strong acid type, sulfonic group) and Chelex 100 (weak acid type, iminodiacetate group), to better understand their potential for selective removal of radium ions (Ra^{2+}) from wastewater such as hydraulic-fracturing produced water. Radium is a highly toxic and radioactive contaminant often co-existing with abundant alkali and alkaline-earth ions, making its selective separation a major challenge.

For Chelex 100 in the sodium form, the selectivity coefficients (K^+/Na^+, Ca^{2+}/Na^+) were determined to evaluate the resin's affinity toward mono- and divalent ions relative to Na^+. For Dowex 50W-X8 in the hydrogen form, the ion pairs K^+/H^+, Na^+/H^+, Ca^{2+}/H^+ were studied to compare the selectivity behavior under strongly acidic conditions. Batch equilibrium experiments were conducted using controlled ionic strengths and metal ion concentrations, followed by analysis of the equilibrated solutions via Ion Chromatography (IC).

The resulting selectivity coefficients will elucidate how resin structure, charge density, and functional group acidity influence ion-exchange preference. Comparing the two resin systems will provide mechanistic insights into the competitive binding of Ra^{2+} with other cations and guide the rational design of efficient ion-exchange or hybrid sorbents for radiological water purification.

Use of the Opentrons Flex Automated Liquid Handling System in Teaching and Research

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Laboratory automation has become an essential tool in both research and industrial settings. Therefore, in order to ensure workforce readiness, undergraduates must be familiar with the use and operation of robotic liquid handling systems. The Department of Chemistry & Biochemistry at JMU obtained an Opentrons Flex liquid handling system in November 2025. The robot includes customizable deck configuration, on-deck labware, automated calibration, and an 8-channel (up to 1000 µL) and a single-channel (up to 50 µL) pipet. The robot can be operated via touchscreen or on the Opentrons application for programmable automation. Here we used the app to develop scripts that demonstrate the robot's volumetric accuracy and precision. Specifically, methods were developed for serial dilutions and to prepare standards for external and internal calibration. This demonstration shows how the Opentrons system may be integrated into teaching and research workflows at JMU.

Mass Spectrometric Validation of Novel Red Pigment Synthesis from Sunflower Flour

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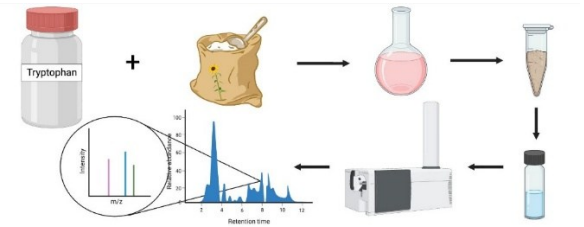

The negative health effects of synthetic dyes, such as red 3, have become increasingly studied over the last decade. As this awareness spreads, consumers demand foods that are free of artificial dyes. This poses a challenge to the food industry, as dyes are used to enhance the visual appeal of foods (e.g., we eat with our eyes first). Subsequently, manufacturers have moved toward the use of natural pigments (e.g., beets or carrots) or the synthesis of dyes from natural precursors. One such synthesis produces a red pigment from the reaction between tryptophan (Trp) and chlorogenic acid (CGA) at high pH. Researchers from Chapman University conducted the same reaction scheme with sunflower flour, which is rich in CGA (0.5-3.6 g CGA per 100g). To validate that this reaction produced the same dye synthesized with the pure reagents, mass spectrometry (MS) was used. Specifically, LC q-TOF was used to obtain exact mass and MS/MS measurements of the target CGA-Trp pigments within the complex sunflower flour matrix. Low concentrations of these pigments were only observed at extremely high sample concentrations (>50 mg/mL). A large unresolved hump, with an absorbance at 550 nm, in the LC chromatogram suggests the production of more (potentially new) red pigments in addition to CGA-Trp. These additional pigments likely result from other phenolic acids present in sunflower flour. Future research will use LC/MS to build a library of these red absorbing analogs to gain more insight into the formation of these pigments and the use of sunflower flour precursor to production of naturally, derived-red pigments.

The Selective Catalytic Epoxidation of Ethylene on Ag/Cu(111)

Katherine B. Weinstock, James T. Whitted, Allen C. Shepherd, Jaimin J. Ashra, Emily M. Euler, David W. Compton, and Dr. Ashleigh E. Baber
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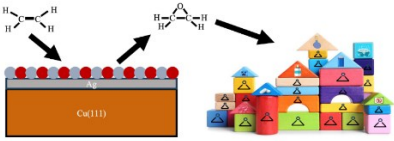

The production of ethylene oxide is a major industrial process that plays an integral role in the formation of insecticides, detergents, adhesives, and other products. Although it is vital, the mass production of ethylene oxide is the fifth-largest producer of CO2, and its synthesis requires dangerous and expensive promoters. Due to this controversial environmental impact, alternative approaches to promoters are being investigated. The use of AgCu catalysts is promising for ethylene epoxidation without the need for promoters. Although the AgCu materials are active for epoxidation, the oxygen species responsible for the reaction remains elusive. To uncover the nature of the oxygen that drives epoxidation rather than combustion, model Cu(111) catalysts were modified with Ag, then oxidized with atomic O to form hydroxyl groups. The products of the reaction of ethylene over hydroxylated and oxidized Ag/Cu(111) were monitored using temperature-programmed desorption (TPD) under ultrahigh vacuum conditions. TPD revealed that hydroxylated Ag successfully suppressed CO2 while simultaneously enhancing the selectivity of ethylene epoxidation.

Propylene Epoxidation via Ice Trapping on Cu-based Surfaces

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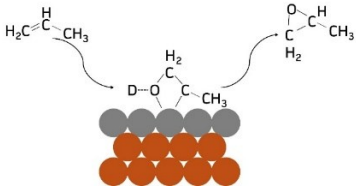

The selective catalytic epoxidation of alkenes using Ag and Cu catalysts are major industrial processes, with value-added products worth a combined $77 billion global market value. Cu-based heterogeneous catalysts are known to enhance propylene (C3H6) epoxidation, but struggle to simultaneously suppress the combustion pathway without the presence of toxic promoters (Cl, Na, Cs). The highly selective epoxidation of various olefins occurs on oxidized Ag(110) and Ag(111), while sequentially limiting the combustion pathway. Ag(111) is not easily oxidized, yet is selective for epoxidation, while Cu(111) readily oxidizes but leads to combustion. By combining these two materials, oxophilic Cu with the epoxide-selective Ag, into a bifunctional AgCu near surface alloy, inadvertent CO2 production could be limited while sustaining propylene oxide formation. Ultra-high vacuum temperature programmed desorption (UHV-TPD) spectra were gathered on partially oxidized Cu(111) and Ag/Cu(111) after dosing propylene. These results showed that atomic O does not lead to selective epoxidation and therefore is not likely the reactive oxygen species of interest. The role of surface-formed hydroxyls for propylene reactivity was explored by conducting TPDs on a H2O/O/Cu(111) surface. H2O is necessary for hydroxyl and ice formation, which traps propylene on the catalytic surface to react at higher temperatures. The combustion and epoxidation pathways were present at high temperatures (~360 K) for the hydroxyl system, but by depositing 1 ML of Ag on Cu(111) via physical vapor deposition, the combustion pathway was fully minimized while retaining the epoxidation pathway. Future work will focus on utilizing scanning tunneling microscopy to image the complex surface and elusive intermediates. Our collaborators will conduct reactor studies to explore scaling the reaction to industrially relevant conditions and computational modeling to create a better understanding of reaction pathways.

Spectroscopic Studies of Environmental Influences on Protein Structure and Stability

Paige O. Wooten and Dr. Gina MacDonald
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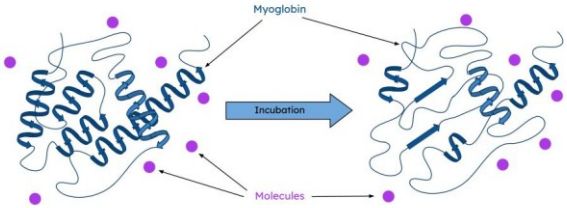

Different environmental influences are known to alter protein structure and stability. Molecules that destabilize protein structure could ultimately lead to increased protein aggregation and promote disease. In contrast, molecules that stabilize proteins can provide insight into the complexity of protein stability and opportunities for treatments to slow aggregation. This study investigates how different molecules affect the structure and stability of the model proteins Myoglobin (Myo) and α-Chymotrypsin (ACT). Spectroscopic studies of the proteins in the presence of Brilliant Blue FCF, Sunset Yellow, glycine, histidine, and caffeine give insight into how these molecules influence protein structure and stability. The food dyes Brilliant Blue FCF and Sunset Yellow as well as glycine, histidine, and caffeine have previously been shown to influence protein structure and/or stability of other proteins. This current study used Fourier-Transformed Infrared (FTIR) and Circular Dichroism (CD) spectroscopies to monitor how the molecules influence protein secondary structure, stability, and aggregation. CD and infrared spectra were obtained on each protein in the presence of each molecule and compared to control samples. In addition, CD spectroscopy was used to monitor how increasing temperature altered protein structures in the presence of each molecule and to determine if the molecules altered protein melting temperatures and aggregation.

2026 Department of Chemistry and Biochemistry Student Award Winners

D.S. Amenta Award	Colin Kress
R.D. Cool Award	Emily Euler
J.W. Chappell Scholarship (May 2025)	Taylor Newman
Palocsay Award in Undergraduate Research (2025)	Hung Quach
Deborah Warnaar & Brian F. Bauer Chemistry Scholarship (2025)	Deborah Emmanuel Reese Secord Josue Santos Santos
Service Award	Rhody Brown
J. W. Chappell Award	Hung Quach
American Institute of Chemists	Peter Henry
Degesch America Award	James Whitted
ACS Award	Olivia Coer
Liberty Casali Memorial Scholarship Fund (2025)	Sara Scanlan
Dean's Award (Chemistry)	Nathan Morris
Dean's Award (Biophysical Chemistry)	Rhett Sanders
CRC First Year Student Award	Wesley Jarrett
Dr. Iona Black Award	Taylor Newman
Inclusive Excellence Award	Caitlin Gutierrez
Goldwater Scholar	Emily Euler
Outstanding Student Researcher Award	*to be announced*

Divisional Awards

ACS Analytical Award	Maxwell Tyree
ACS Biochemistry & Chemical Biology Award	Sara Scanlan
ACS Environmental Award	Luke Campbell
ACS Inorganic Award	Sara Scanlan
ACS Organic Award	Anna Grove
ACS Physical Award	Elaina Manyin

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