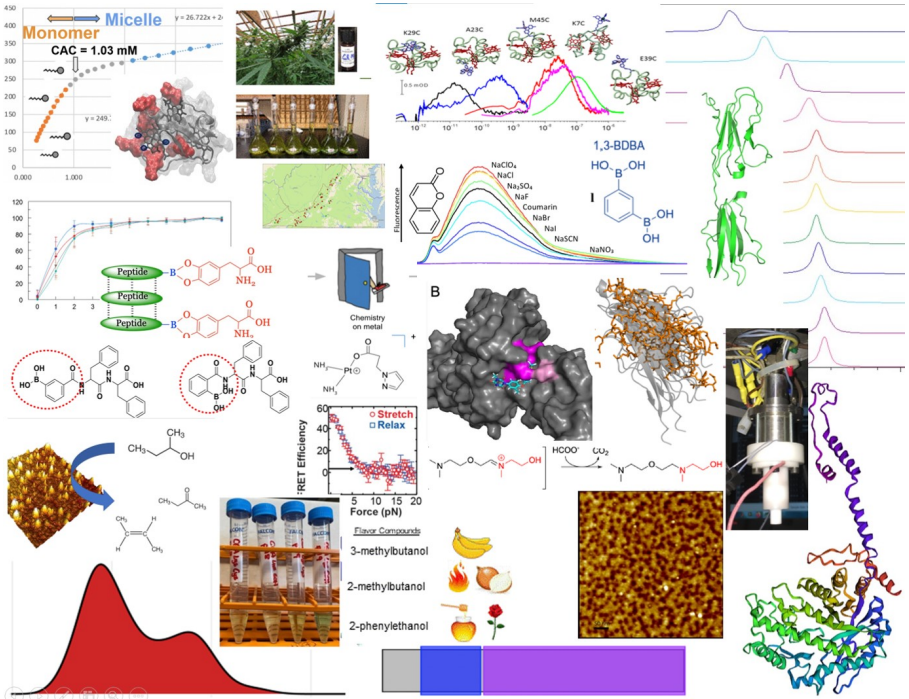
JAMES MADISON UNIVERSITY

DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY



46TH ANNUAL SPRING UNDERGRADUATE RESEARCH SYMPOSIUM

THURSDAY APRIL 21, 2022

ORAL SESSION I: 1:30 – 2:30 PM (ENGEO 1301)
POSTER SESSION: 4:00 – 5:00 PM (PCB LOBBY)

FRIDAY APRIL 22, 2022

ORAL SESSION II: 2:30 – 3:45 PM (ENGEO 1301)
SPECIAL ANNOUNCEMENTS: 3:55PM (ISAT 159)
KEYNOTE ADDRESS: 4:00 – 5:00 PM (ISAT 159)

46th Annual Department of Chemistry and Biochemistry
Spring Undergraduate Research Symposium

Keynote Speaker

Timothy W. Graul, PhD
(JMU Class of 1994)
Director in the Global CMC Advisory Office
Pfizer Inc.
Groton, CT

Timothy W. Graul is a Director in the Global CMC Advisory Office within Pfizer Inc at the Groton, CT site. He received his Bachelor of Science Degree in Chemistry at James Madison University and then Ph.D. in Analytical Chemistry at The Florida State University under the direction of Joseph B. Schlenoff. After completing studies, Tim joined Pfizer and supported the development of drug product formulations and drug substance synthetic routes by providing analytical methods, data, and strategy as a member of Analytical R&D. He has been fortunate to have contributed to the filing, registration, and successful approval of a number of life-changing products. During his time at Pfizer, Tim has been recognized as a leader in Quality by Design for analytical methods. He has collaborated on publications that have been at the forefront of industry in this area. He was recently appointed as the PhRMA Deputy Topic lead on the ICH Q2/Q14 (Validation of Analytical Procedures and Analytical Procedure Development) Expert Working Group. He also expanded his influence by being engaged in industry efforts for global harmonization in the submission and acceptance of process and product control strategies.

Tim has been a member of industry groups including Land O' Lakes Pharmaceutical Analysis Conference Planning Committee since 2010 (where he was the Chair for the 2016 Conference and awarded the Mel Weinswig Award for his contributions to the conference), IQ groups such as Analytical Leadership, AQbD, Dissolution, Control Strategy Harmonization Metrics, and Worldwide Specification Harmonization.

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
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 21, 2022 *(EnGeo 1301)*

1:30 pm	Grace Moncure, Dr. Nathan Wright, and Dr. Callie Miller	The N-terminus of obscurin exhibits significant flexibility in solution
1:45 pm	Gianna E. Mauriello, Dr. Callie J. Miller, and Dr. Nathan T. Wright	The N-terminus of obscurin exhibits significant flexibility in solution
2:00 pm	Samantha L. Forbes, Rachel J. Stegmeier, Dawson D. Bowles, and Dr. Daniel M. Downey	Analysis of Commercial Extraction of Phytocannabinoids from Hemp
2:15 pm	Liv C. Mumma and Dr. Yanjie Zhang	Coumarin Fluorescence in the Presence of Hofmeister Anions

Poster Session: Thursday April 21, 2022, 4:00 – 5:00 pm *(PCB lobby)*

Roujon Aranowzari, Isabel M. Romov, Nathan T. Wright	Searching for a Molecular Bandaid: Preventing Protease Cleavage of Desmoplakin Mutants
Rhen Blake, Nicole Wilson, James Clifford, Amanda McKee, Max Weinsweig, Eli Wojdyla, Andrew Jaycox, Tyler Miller, Brenden Wimbish, and Dr. Kevin L. Caran	Studies on the Relationship Between Amphiphile Chain Length and Aggregation
Christine N. Buchholz, Abigail E. Sholes, Raymond A. Enke, and Christopher E. Berndsen	Structural characterization of the cone-rod homeobox protein binding to DNA
Samuel L. Dimitri, Dr. Paul L. Raston, and Dr. Chakree X. Tanjaroon	Development of High Voltage Pulser Instrument for Microwave Spectrometer
Camryn S. Dudek and Dr. Christopher Berndsen	Purifying Plastics to Prevent Pollution, a Method for Cleaning Single-use Micropipette Tips
Kurt B. Espinosa, S. Maddie Beck, JJ N. Fitzhenry, Jonathan M. Schmitz and Dr. Linette M. Watkins	Kinetic and Stability Study on the Immobilized Enzymatic Step of One-Pot Dimerization of 2-[2-(dimethylamino)ethoxy]ethanol
Lyssa A. Garber, Ava. J. Galgano, Clayton J. Rogers, and Dr. Ashleigh Baber	Reactivity of Butanol on TiO_2/Au(111) Inverse Model Catalysts
Sophia Gross, Tyler Brittain and Dr. Oleksandr Kokhan	Biophysical characterization of metal binding in the Ppc family
Angela J. Kayll, Gabriella M. Newsome, and Christopher E. Berndsen	Structural Modeling and Characterization of a Putative β-amylase 9 from *Zea mays*
Stephan Michaelov and Dr. Daniel Downey	Acid/Base Status and Water Chemistry of Headwater Streams in VA's National Forest
Trinity S. Perry, Kathy Elliot and Dr. Isaiah Sumner	The Role of pK_a Suppression in the Ubiquitination Reaction
Stuart A. Regitz, Daniel P. Musikanth, Ryan T. Johnson, Dr. Donna S. Amenta and Dr. John W. Gilje	Synthesis of N-Pyrazolylpropanoate Derivatives as Potential Ligands with Palladium
Andrew M. Roberts, Lynnea Gedney and Dr. Christine Hughey	Monitoring compounds involved with CGA-Lys greening in alkaline reaction mixtures
Clayton Rogers, Chris A. Whitehouse, Dr. Christina M. Rost, Dr. Ashleigh E. Baber	Surface Morphology Evolution of $(MgNiCoCuZnCr)_{0.167}O$ Thin-Films
Zachary D. Ryan and Dr. Oleksandr Kokhan	Rational Design of Ultrafast PpcA-Ru$(bpy)_3$ Complexes
Leighann R. Weber, Amanda Cicali, Lynn E. Marsh, Steven Harper, Dr. Samuel A. Morton, and Dr. Christine A. Hughey	Evolution of Metabolites in a Single Malt, Single Hop (SMaSH) Beer Using Targeted and Untargeted Analysis
Paul M. Wilson and Dr. Gretchen M. Peters	Boronic Acid Orientation Effects on Hybrid Peptide-Polymer Properties

(Student presenters underlined)

Oral Session II: Friday April 22, 2022 *(EnGeo 1301)*		
2:30 pm	James Clifford, Rhen Blake, Nicole Wilson, Max Weinsweig, Amanda McKee, Eli Wojdyla, Andrew Jaycox, Tyler Miller, Brenden Wimbish and Dr. Kevin L. Caran	Ammonium Based Tris-Cationic Amphiphiles: Colloidal Aggregation
2:45 pm	Ani N. Davis and Dr. Gretchen M. Peters	The Characterization of Isomeric Diboronic acid Crosslinker additions to PVA-BA Organogels as a Model for a Stimuli Responsive Gel System
3:00 pm	Isaac D. Peregoy and Dr. Gretchen M. Peters	Triphenylamine Boronic Acid Gels For L-DOPA Delivery
3:15 pm	Abigail N. Collins, Quinn C. Harkrider, C. Jackson White, Dr. Nathan T. Wright, Dr. Kristopher Kubow, and Dr. Daniel E. Conway	Modulating Obscurin's Force Sensation in Epithelial Cells
3:30 pm	Rachel J. Stegmeier, Samantha Forbes, and Dr. Daniel Downey	Statistical Analyses of Hemp and Hemp Product Cannabinoid Test Results

(Student presenters underlined)

Special Announcements *(ISAT 159)*	
3:55pm	Announcement of Chemistry and Biochemistry Student Award Winners

Keynote Address: Friday April 12, 2019 *(ISAT 159)*		
4:00 - 5:00 pm	Timothy W. Graul, PhD JMU Class of 1994	Stream Water Chemistry to Development of Pharmaceutical Synthetic Routes and Formulations

Keynote Address

Friday, April 22, 2022 at 4:00pm
ISAT Room 159

Stream Water Chemistry to Development of Pharmaceutical Synthetic Routes and Formulations

Timothy W. Graul, PhD
(JMU Class of 1994)
Director in the Global CMC Advisory Office
Pfizer Inc.
Groton, CT

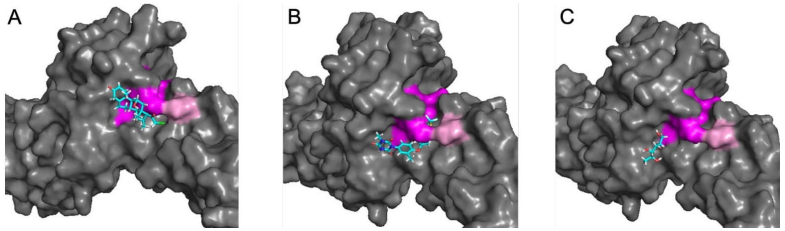
Analytical chemists play an integral role in the development of pharmaceutical synthetic routes and formulations. They support all phases of development from pre-clinical toxicology studies through commercial launch. The process for developing analytical methods to support clinical and commercial products will be presented with a focus on forced degradation studies that are used to identify potential degradation products in active pharmaceutical ingredients and pharmaceutical formulations. Knowledge gained from these studies allows analysts to understand the intrinsic stability of the active pharmaceutical ingredient, underpin method development and validation of stability indicating methods, and aid in determining pharmaceutically relevant degradant pathways which can provide insight into control strategies that can ensure stable material throughout shelf life. Further, alignment across industry of study design for forced degradation studies is discussed. From this alignment, leading experts from pharmaceutical companies have engaged with Brazilian health authorities on the scientific merits of specific forced degradation conditions in Brazilian regulations that are not likely to generate relevant degradation products. Advocacy efforts such as these are aimed at reducing the resource and cost burden of developing new drugs. The presenter will share his journey as an analytical chemist that began with undergraduate research at James Madison University and has led to supporting the development of life-changing therapeutic products.

STUDENT ABSTRACTS

(Student presenters underlined)

Searching for a Molecular Bandaid: Preventing Protease Cleavage of Desmoplakin Mutants

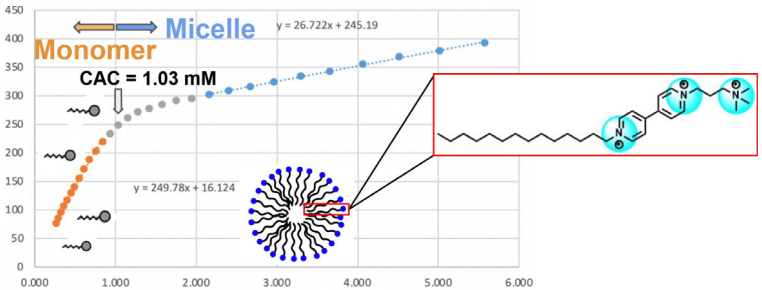
Roujon Aranowzari, Isabel M. Romov, Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



The desmosome is a protein complex that connects the intermediate filament network of one cell to that of its neighboring cell. Crucial for cell-cell adhesion, it is most often found in tissues that undergo mechanical stress, such muscular and cutaneous tissue. One protein integral to the desmosome is the intermediate filament binding protein, desmoplakin (DSP). Multiple missense mutations around 299-515 residue range of DSP have correlated with desmosome-related diseases, such as arrhythmogenic cardiomyopathies. This is surprising, since this section of the protein neither binds to other desmosomal protein nor binds to intermediate filaments. Furthermore, both molecular modeling and circular dichroism experiments show that clinically significant DSP mutants maintains their structural integrity. Yet, these mutants result in decreased cellular DSP levels. Previous work in our lab provided a molecular mechanism for this apparent contridiction; mutations in this region expose a previously-occlued calpain cleavage site (residues 447-451). Thus to rescue DSP, one can simply block calpain-dependent DSP degradation. Instead of inhibiting calpain, a protease necessary in calcium-dependent processes, we aim to find a “molecular band-aid” for DSP: a molecule that blocks this cleavage site. Through both in-silico simulations and in-vitro fluorescence assays, we have identified multiple FDA-approved drug candidates that bind to DSP and prevent protease-mediated degradation.

Studies on the Relationship Between Amphiphile Chain Length and Aggregation

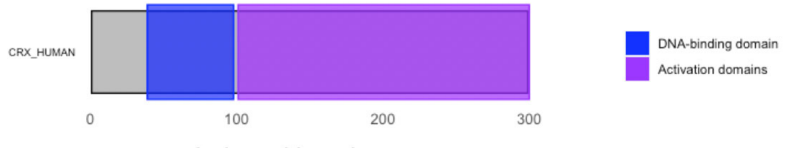
Rhen Blake, Nicole Wilson, James Clifford, Amanda McKee, Max Weinsweig, Eli Wojdyla, Andrew Jaycox, Tyler Miller, Brenden Wimbish, and Dr. Kevin L. Caran
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



In order to develop a better understanding of the relationship between an amphiphile’s structure and its capacity to aggregate, we have prepared a new series of tris-cationic amphiphiles. The amphiphiles in the new series (3-3-N-BIPY-R) each have a bis-pyridinium core with a propyl trimethyl ammonium group on one side and varying hydrocarbon chain lengths on the other side. Amphiphiles with linear hydrocarbon chain lengths of 14, 16, 18, and 20 carbons were synthesized and purified. Nuclear magnetic resonance (NMR) and conductivity were utilized in colloidal studies to determine each molecule's critical aggregation concentration (CAC). These studies provide insight into the relationship between a molecule’s chain length and its CAC.

Structural characterization of the cone-rod homeobox protein binding to DNA

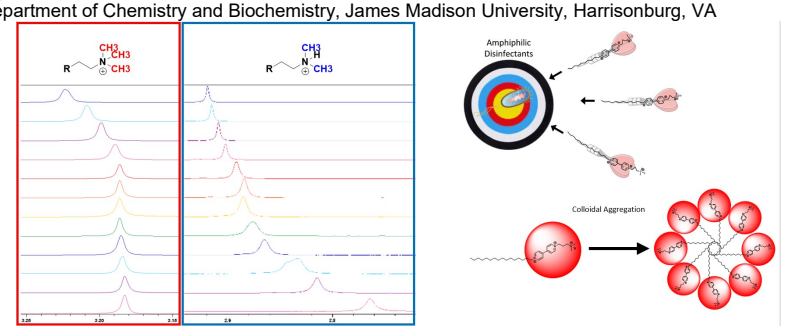
Christine N. Buchholz[1], Abigail E. Sholes[1], Raymond A. Enke[2], and Christopher E. Berndsen[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Biology, James Madison University, Harrisonburg, VA



Roses are red, some eyes are blue, you wouldn’t see this without CRX too. The Cone-Rod Homeobox protein or CRX is an essential transcription factor for the development of cells in the eye called photoreceptors. Photoreceptor cells (PRs) convert light into signals that the brain can understand. CRX plays a role in the differentiation of these photoreceptors into rods and cones, which detect achromatic and colored light, respectively. While there are details known about the molecular function of CRX, there is little known about the structural information of the protein. It is known that CRX contains a DNA binding domain (DBD) and two activation domains (ADs). Changes to the amino acid sequence in any of these regions are linked to a number of diseases associated with congenital blindness. We would like to better understand the structure and function of the AD and DBD to describe the regulation of photoreceptor development by CRX. We used Small-Angle X-Ray Scattering (SAXS) and DNA binding assays on the DBD showing that the DBD is globular and can bind to DNA in the absence of the activation domain. We crosslinked the DBD peptide to DNA with glutaraldehyde in an attempt to get a bound structure of the peptide-DNA complex. The peptide-DNA complex will show more accurately how the DBD binds to DNA and the stoichiometry of the complex. We are working to confirm preliminary findings suggesting a 2:1 DBD:DNA complex. These experiments will help us to understand the role that CRX plays in regulating transcriptional networks in PR neurons.

Ammonium Based Tris-Cationic Amphiphiles: Colloidal Aggregation

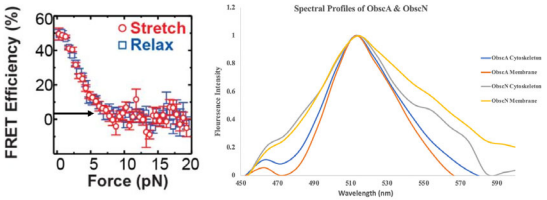
James Clifford, Rhen Blake, Nicole Wilson, Max Weinsweig, Amanda McKee, Eli Wojdyla, Andrew Jaycox, Tyler Miller, Brenden Wimbish and Dr. Kevin L. Caran
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



In this project, we prepared two series of aromatic, triscationic, nitrogen-based amphiphiles for surface sterilization. Each of the two series has a bis-pyridinium core with hydrocarbon chains ($C_{10}H_{21}$ - $C_{20}H_{41}$) attached to one side. On the other side, attached via a linear 3C linker, one series has a dimethyl ammonium group, and the other series has a trimethylammonium group. The molecules were studied using nuclear magnetic resonance (NMR) and conductivity to measure the critical aggregation concentration (CAC). Comparison of CAC values within each series provides information about the relationship between chain length and aggregation. Comparison of CAC values between the two series provides information about the relationship between head group architecture (tertiary vs. quaternary ammonium) and aggregation.

Modulating Obscurin's Force Sensation in Epithelial Cells

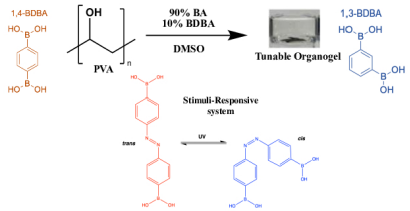
Abigail N. Collins*[1], Quinn C. Harkrider*[1], C. Jackson White*[1], Dr. Nathan T. Wright[1], Dr. Kristopher Kubow[2], and Dr. Daniel E. Conway[3] (*indicates equal contribution)
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA
[2]Department of Biology, James Madison University, Harrisonburg, VA
[3]Department of Biomedical Engineering, Virginia Commonwealth University, Richmond, VA



Obscurin is a giant (720-900 kDa), cytoskeletal protein involved in cell mobility and adhesion signaling. In skeletal muscles where obscurin is typically characterized, it is the only known protein to link the sarcomere to the sarcoplasmic reticulum. In epithelial cells, obscurin regulates cell division, migration, and tension through RhoA pathways. Given that the isoforms of obscurin are similar in both cell types, we suspect obscurin is performing similar molecular tasks, but with different cellular outcomes. While the downstream pathway of obscurin has become gradually clearer in recent years, the mechanism of obscurin regulation has yet to be determined. To wit, no molecule that binds to and activates obscurin to regulate its biological activity has been discovered. Our lab proposes that obscurin is not regulated through biochemical means, but instead by the mechanical forces that obscurin itself regulates. To test this hypothesis, we first need to establish if, and under what conditions, obscurin is under tension. Our data show that obscurin localizes by the membrane, particularly in subcellular areas that are thought to be under tension. To determine if obscurin itself is directly under tension, we expressed several constructs of obscurin containing a FRET-based force sensor in Madin-Darby Canine Kidney (MDCK) cells. Fluorescence intensity analysis shows that obscurin is, in fact, under significant tension, ~5pN, in resting tissue culture. The addition of the actin-disrupting drug cytochalasin D decreases the FRET efficiency of obscurin, and therefore its tension. Together, these findings bolster our hypothesis that obscurin is a novel mechanosensor.

The Characterization of Isomeric Diboronic acid Crosslinker additions to PVA-BA Organogels as a Model for a Stimuli Responsive Gel System

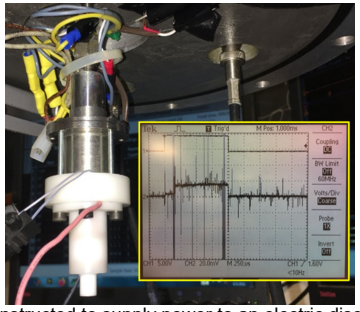
Ani N. Davis and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Polymer gels are a versatile material that has a multitude of applications from biomedical uses like artificial skin to environmental cleanup like toxic waste removal. To form gels, polymer chains must be crosslinked to create a fibrous gel network. Characterization of polymer crosslinking in gel networks allows for the manipulation and optimization of the gel materials. In previous research, we found that boric acid (BA) crosslinks within polyvinyl alcohol (PVA) organogels can be enhanced in the presence of small amounts of 1,4-benzene diboronic acid (1,4-BDBA). With mixtures of BA and 1,4-BDBA, we observed improvements in the rheological and thermal properties, gelation times, and critical gelation concentrations (CGC). We found that 1,3-benzene diboronic acid (1,3-BDBA), the c-shaped isomer of 1,4-BDBA, did not have the same material enhancing effects. Namely, at concentrations lower than its CGC, the addition of 1,3-BDBA has little impact on the storage modulus (Gâ€²) of the PVA/BA gel and no new crosslinks formed. Thus, these findings indicate that the shape and linearity of the diboronic acid impact the efficiency of crosslinking in PVA-BA gels. Interestingly, both BDBA additions to PVA/BA gels had similar recoverability after being placed under stress. Using these two diboronic acids (BDBA) as model systems, we designed a boronic crosslinker, azobenzene-4'4-diboronic acid (ABDBA), that would be able to switch between these two conformations from exposure to UV light. The addition of ABDBA would allow for a PVA/BA gel to change material properties by being triggered by an external stimulus while still having enhanced recoverability properties.

Development of High Voltage Pulser Instrument for Microwave Spectrometer

Samuel L. Dimitri, Dr. Paul L. Raston, and Dr. Chakree X. Tanjaroon
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



A high-voltage pulser was constructed to supply power to an electric discharge source for a chirped pulse Fourier transform microwave spectrometer at Missouri S&T. The pulser was developed from design notes and circuit diagrams that were obtained from a Harvard engineer. The main components of the high-voltage pulser are low voltage and high-voltage circuit boards that connect to the front and back panels, respectively, as well as a fan and power supply. The instrument was used during the summer of 2021 at Missouri S&T to study atmospherically relevant complexes involving the hydroxyl radical (OH). We managed to observe OH-H_2O with very good signal-to-noise, and in future experiments, we plan to use the instrument to produce larger clusters of OH-H_2ON in order to investigate the solvation environment of OH. The real-world application of this research is to understand how atmospherically important radicals dissolve in cloud particles.

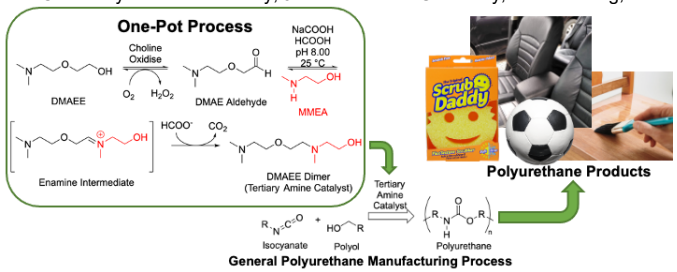
Purifying Plastics to Prevent Pollution, a Method for Cleaning Single-use Micropipette Tips

Camryn S. Dudek and Dr. Christopher Berndsen
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA

There are many types of single-use plastic labware; tubes, cuvettes, containers, and pipettes are just a few of that plastic. During the COVID-19 pandemic, many of these plastics were extremely difficult to get a hold of. My research project aims to find a way to potentially cut down that plastic consumption and reuse one of the most common in Biochemistry labs, pipette tips. In an effort to move forward to more eco-friendly chemistry, this project is utilizing the reuse of pipette tips that are normally disposed of after one use. What this research illuminates is how to effectively reuse the pipette tips by rinsing them to eliminate contamination from prior use in an EtOH bath and then run through an autoclave. The micropipette calibration after each autoclave shows that these tips dispense the same amount of volumes for two different pipette sizes of15µL and 500µLafter being put through the autoclave at 327K for 54 minutes. Not only that but it can continue to be used multiple times through an autoclave with this cleaning method. While certain precautions would have to be taken in the lab to differentiate which pipette tips could be reused due to this not being found to eliminate contamination for tips handling DNA. It would still be a viable way to reuse tips for various chemicals. These findings can help recycle micropipettes tips and help for a better future in green chemistry and cutting down plastic use.

Kinetic and Stability Study on the Immobilized Enzymatic Step of One-Pot Dimerization of 2-[2-(dimethylamino)ethoxy]ethanol

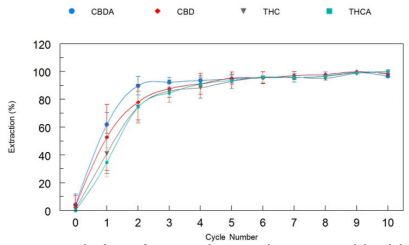
Kurt B. Espinosa, S. Maddie Beck, JJ N. Fitzhenry, Jonathan M. Schmitz and Dr. Linette M. Watkins
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Tertiary amine catalysts (TACs) are essential organic molecules used in polyurethane manufacturing. Synthesis of these chemicals involves the use of catalytic transition metals at high temperatures and high pressures. Simple amine systems react easily with transition metals; however, amine systems with multiple hydroxyl groups and methylamine complexes produce significant byproducts. In this study, synthesis that forgo transition metals is explored. Enzymes can provide a clean industrial alternative to transition metal use. 2-[2-(dimethylamino)ethoxy]ethanol (DMAEE) is the monomer used in the synthesis of a model TAC. When DMAEE is first enzymatically oxidized, the aldehyde can serve as an electrophile for 2-(methylamino)ethanol (MMEA), forming the DMAEE dimer. Choline oxidase catalysis is the first step of this pathway. Steady state kinetic parameters of choline oxidase with choline and DMAEE as substrates, optimum pH, and temperature stability are reported in this study. The effect of MMEA on the enzymatic reaction is examined as well. In an industrial application, immobilized enzymes can enhance stability over a broad range of temperature and pH. Therefore, choline oxidase was immobilized on CNBr-activated Sepharose beads, and the effects of immobilization are reported in this study.

Analysis of Commercial Extraction of Phytocannabinoids from Hemp Biomass

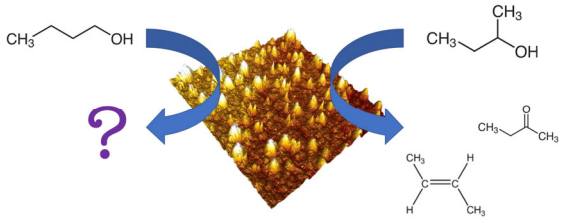
Samantha L. Forbes, Rachel J. Stegmeier, Dawson D. Bowles, and Dr. Daniel M. Downey
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Cannabis sativa (hemp) is an annual plant that produces phytocannabinoids for protection from UV light and strong winds, along with hundreds of other chemicals. The phytochemicals have alleged medical benefits and must be separated from the plant biomass for the manufacture of drugs and dietary supplements by passing a solvent through a bed of finely ground dried plant material. The solvent is removed after the extraction process to produce a viscous dark liquid known as crude oil. We have examined three popular commercial extraction technologies: single pass ethanol, multi-pass ethanol, and supercritical fluid CO_2 for efficiency, yield, and throughput. The increase of cannabinoid concentrations following each cycle for the multi-pass ethanol was monitored. Data were collected on cannabinoid concentrations in hemp biomass and crude oil for all three extraction technologies. High-Pressure Liquid Chromatography Ultraviolet Detection (HPLC-UV) and Gas Chromatography Flame Ionization Detection (GC-FID) were used for analyses primarily for cannabidiol (CBD), cannabidiolic acid (CBDA), Δ-9-tetrahydrocannabinol (THC), and Δ-9-tetrahydrocannabinolic acid (THCA). Multi-pass extraction was the most effective technology for removal of the phytocannabinoids. For multi-pass extractions of up to ten cycles steady state was achieved within five cycles with most extraction by the third cycle. This observation reduces time, labor, and energy for commercial ethanol extraction.

Reactivity of Butanol on TiO_2/Au(111) Inverse Model Catalysts

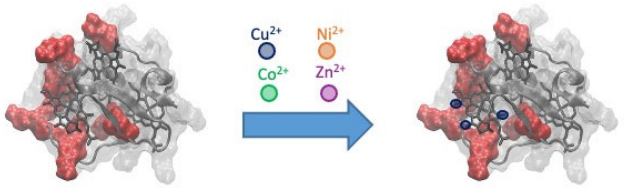
Lyssa A. Garber, Ava. J. Galgano, Clayton J. Rogers, and Dr. Ashleigh Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Biofuels can be used to reduce global dependence on fossil fuels while contributing to a carbon-neutral cycle. Biobutanol has low volatility and multiple transportation options making it an attractive alternative fuel. To better understand how butanol breaks down in heterogeneous catalytic processesâ€š temperature programmed desorption (TPD) is used to investigate its reaction on TiO_2/Au(111). Inverse model catalysts of interest were formed by depositing TiO_2 nanoparticles onto Au(111) using physical vapor deposition. Low temperature desorption features help to understand how the molecule adsorbs to the surface while the high temperature peaks are used to understand chemical reactivity and selectivity. Low temperature peaks indicate different molecular packing of 1-, 2-, and i-butanol. The major high temperature products from the reaction of 2-butanol on TiO_2/Au(111) are 2-butanone and butene observed at ~500 K. The selectivity of the reaction was not altered during successive desorption experiments, indicating that the model catalyst was stable without reoxidation between experiments. Preliminary studies of the reaction of 1-butanol and isobutanol indicate that both reduced and oxidized products are formed, but need to be further studied to identify the species and stability. Atomic force microscopy (AFM) images show that the inverse model catalyst has ~0.16 ML of TiO_2 dispersed across the Au(111) surface in predominantly 1D nanoparticles. Early studies of butanol on TiO_2/Au(111) suggest that the structure affects the reactivity and stability of butanol at high temperatures.

Biophysical characterization of metal binding in the Ppc family

Sophia Gross, Tyler Brittain and Dr. Oleksandr Kokhan
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Dissimilatory metal-reducing bacteria utilize metal ions and metal oxides instead of oxygen in their respiration. Metal-reducing bacterial genomes are very rich (>100) in genes encoding multiheme cytochromes. However, the exact molecular pathways linking cytosolic redox reactions to periplasmic cytochromes and extracellular electron acceptors are not clear. Here we demonstrate with isothermal calorimetry (ITC) that PpcA, the most abundant periplasmic cytochrome in Geobactur sulfurreducens, binds Cu^{2+} with 1:1 stoichiometry and sub-uM affinity. However, no binding was observed with the other metals from Irving-Williams series. Using 1D and 2D NMR we identified the surface area responsible for Cu^{2+} binding. Sequence conservation analysis suggests that the other members of the Ppc family are likely to bind Cu^{2+}.

Structural Modeling and Characterization of a Putative β-amylase 9 from *Zea mays*

Angela J. Kayll, Gabriella M. Newsome, and Christopher E. Berndsen
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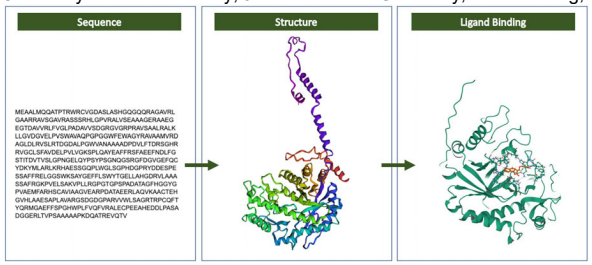

Photosynthesis occurs throughout the day, producing glucose that then can be stored as starch or used as energy in plants. **β**-amylases, or BAMs, are protein enzymes that typically degrade starch in plants to produce a sugar known as maltose (Monroe & Storm, 2018). Our project aims to discover the structure of a specific BAM variant. Knowing information about the structure can lead to information about the functionality of our structure, which can give insight into the uses of BAMs in humans and plants. The BAM protein that we believe our sequence to be of specifically is from the *Zea mays* variant of BAM9, which has not been studied in depth. Using the homology modeling software trRosetta, SWISS, and Phyre[2], we analyzed our given sequence to predict the structure. Further structural assessments of our models were performed using programs such as IUPred2A, PrDOS, and MolProbity. Molprobity analysis of our models allowed us to determine the prediction accuracy through methods such as disorder prediction, clashscore, molprobity score, and Ramachandran outliers. Mol* was also used to compare our structures against a known ligand-containing model that was similar to ours. Through this, similarities and differences in amino acid sequences and weak interactions to the ligand were observed. We compared the active site of our BAM to the active site of a known BAM5 with amylase activity, finding that our BAM9 variant is inactive by structural comparison. We then docked a small library of plant metabolites to the predicted BAM9 to determine ligand binding and identify potential cellular functions. For this analysis, we then proposed a potential inhibitor of our protein and determined how it would bind to our BAM9. Finding all of this information will allow for a proposal of the cellular function of BAM9, and how this could potentially link in plant function.

The N-terminus of obscurin exhibits significant flexibility in solution

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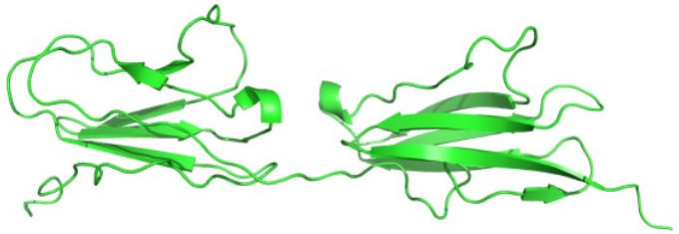

The N-terminal half of the giant cytoskeletal protein obscurin is comprised of more than 50 Ig-like domains, arranged in tandem. Domains 18-51 are connected to each other through short 5-residue linkers, and this arrangement has been previously shown to form a semi-flexible rod in solution. Domains 1-18 generally have slightly longer ~7 residue interdomain linkers, and the multi-domain structure and motion conferred by this kind of linker is understudied. Here, we use NMR, SAXS, and MD to show that these longer linkers are associated with significantly more domain/domain flexibility, with the resulting multi-domain structure being moderately compact. Further examination of the relationship between interdomain flexibility and linker length shows there is a 5 residue ‘sweet spot’ linker length that results in dual domain systems being extended, and that either longer or shorter linkers compacts the overall structure. These insights allowed us to more fully explore how obscurin behaves in solution. Modelling of domains 1-18 suggests that this region can form tangles. Given how infrequently protein tangles occur in nature, and given the pathological outcomes that occur when tangles do arise, our models suggest that obscurin is likely either significantly scaffolded or else extended in the cell.

Acid/Base Status and Water Chemistry of Headwater Streams in VA’s National Forest

Stephan Michaelov and Dr. Daniel Downey
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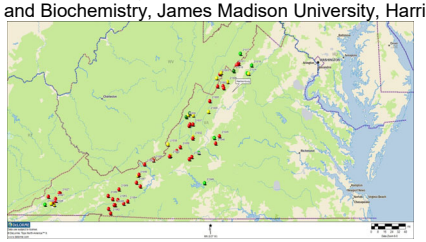

Every year, the US Forest Service conducts a synoptic sampling of the George Washington and Jefferson National Forests for water chemistry analyses of the streams by the James Madison University (JMU) Environmental Chemistry Group. This year, 67 samples were collected from Northwestern Virginia to the southern Tennessee-Virginia border. Samples were then delivered to James Madison University for assessment. Weathering of geologic material upstream of sample collection sites provides the chemical components of the water. Samples were analyzed for pH, acid neutralizing capacity (ANC), conductivity, and concentrations of sodium, potassium, calcium, magnesium, chloride, nitrate, sulfate and aluminum. These parameters were selected as they enable water chemists to describe the health of a stream and potential toxicity for fish, especially brook trout (Salvelinus fontinalis). High pH (>5.5) and ANC (>2 ppm) streams are able to withstand acid rain deposition and protect fishes from substantial pH changes. Low pH (<5.5) streams typically have high concentrations of aluminum (>100 ppb), which is acutely toxic to fish as it interferes with the function of their respiratory system. Data were interpreted by analyzing the geological features of each sample site. Low pH samples had geological composition of primarily sandstone (silica oxide) which provides virtually no base buffers for the stream. Mid to high pH samples show the effects of geological composition change from sandstone to limestone/dolomite (calcium/magnesium carbonate) as the carbonate provides base buffer to the streams. The stream data collected each year aids US Forest Service planning of acid mitigation practices, i.e. liming, controlled fire burns and forest timber harvesting.

The N-terminus of obscurin exhibits significant flexibility in solution

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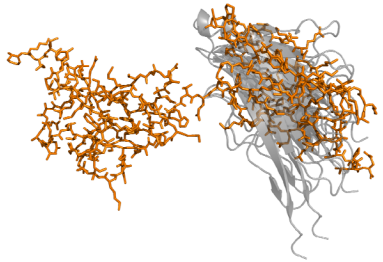

The N-terminal half of the giant cytoskeletal protein obscurin is comprised of more than 50 Ig-like domains, arranged in tandem. Domains 18-51 are connected to each other through short 5-residue linkers, and this arrangement has been previously shown to form a semi-flexible rod in solution. Domains 1-18 generally have slightly longer ~7 residue interdomain linkers, and the multi-domain structure and motion conferred by this kind of linker is understudied. Here, we use NMR, SAXS, and MD to show that these longer linkers are associated with significantly more domain/domain flexibility, with the resulting multi-domain structure being moderately compact. Further examination of the relationship between interdomain flexibility and linker length shows there is a 5 residue â€˜sweet spotâ€™ linker length that results in dual domain systems being extended, and that either longer or shorter linkers compacts the overall structure. These insights allowed us to more fully explore how obscurin behaves in solution. Modelling of domains 1-18 suggests that this region can form tangles. Given how infrequently protein tangles occur in nature, and given the pathological outcomes that occur when tangles do arise, our models suggest that obscurin is likely either significantly scaffolded or else extended in the cell.

Coumarin Fluorescence in the Presence of Hofmeister Anions

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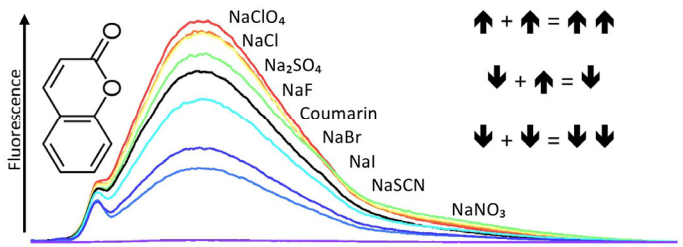

The Hofmeister series is a list of ions first discovered in 1888 by Franz Hofmeister that ranks ions' ability to influence protein-aggregation, -folding, -solubility, and enzyme activity. A fluorescence of a model drug, coumarin, was monitored in the presence of a series of sodium salts with anions in the Hofmeister series. Kosmotropic SO_4^{2-}, F^-, Cl^- and chaotropic ClO_4^- increased the fluorescence intensity of coumarin. Chaotropic Br^-, NO_3^-, SCN^-, and I^- quenched the fluorescence of coumarin. The Stern-Volmer equation was used to model the anions' ability to change the fluorescence of coumarin at 20 and 50 °C. The effects of mixed ions quenching were also investigated. The combination of two fluorescence enhancing ions increased the fluorescence of coumarin in an additive manor. The combination of two fluorescence quenching ions decreases the fluorescence of coumarin more than each individual ion but in non-additive manors. When a fluorescence enhancing ion is combined with a quenching ion, the quencher ion dominates the process and the fluorescence of coumarin appears to be like the quencher ion in solution alone. Temperature dependence of coumarin fluorescence was investigated in the presence of combined ion pairs and the results mirrored that of the trials at different ion concentrations.

Triphenylamine Boronic Acid Gels For L-DOPA Delivery

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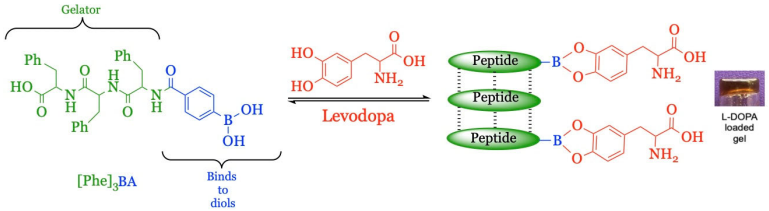

The ability to deliver drugs to specific locations in the body and release them in a controlled fashion is critically important for patient outcomes and drug efficacy. Supramolecular gels are highly attractive for such drug delivery applications, as they are generally biocompatible and stimuli-responsive. Herein, we report a peptide-based supramolecular gelator with a boronic acid handle ([Phe]3BA) designed to target and reversibly release the Parkinson's disease drug levodopa (L-DOPA). NMR titrations and alizarin red S fluorescence assays indicate [Phe]3BA readily binds to L-DOPA via boronate ester linkages. Furthermore these ester linkages are maintained upon [Phe]3BA gelation. This L-DOPA loaded gel has potential as a controlled and targeted release system for L-DOPA.

The Role of pK_a Suppression in the Ubiquitination Reaction

Trinity S. Perry, Kathy Elliot and Dr. Isaiah Sumner
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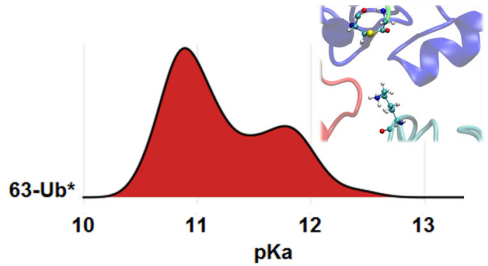

Ubiquitination is an important chemical reaction in our cells and is responsible for a variety of processes like DNA repair and protein degradation. Ubiquitination is a three-step reaction catalyzed by three enzymes, a ubiquitin-activating enzyme (E1), a ubiquitin-conjugating enzyme (E2) and a ubiquitin ligase enzyme (E3). These enzymes work together to bind a ubiquitin to a lysine residue on a specific protein by an iso-peptide bond. The first step in this reaction is the removal of a proton from the target lysine. If the lysine is not deprotonated, this can lead to disruptions in the Ubiquitination process potentially causing cancer, neurodevelopmental issues, and diseases. There are currently two hypotheses regarding the mechanism of proton removal – active and passive deprotonation. In the active mechanism, there are two well conserved acidic residues that can serve as conjugate bases to remove the proton from the lysine. In the passive mechanism, deprotonation occurs when the active site decreases the pKa of the substrate lysine. It is also possible there is no universal mechanism describing this proton removal. This research project focuses on the deprotonation mechanism used by the E2, Ubc13. Ubc13 forms polyubiquitin chains (i.e. it ubiquitinates ubiquitin). Since the mechanism is poorly understood for Ubc13, we tested both hypotheses using computer simulations. We used electronic structure theory to test the active mechanism and we used molecular dynamics simulations to determine the passive mechanism, specifically, we analyzed the pK_a of the lysine using the PropKa software. Our results indicate that the pK_a of lysine does not appreciably change when it interacts with Ubc13, which shows that Ubc13 may favor the active mechanism.

Synthesis of N-Pyrazolylpropanoate Derivatives as Potential Ligands with Palladium

Stuart A. Regitz, Daniel P. Musikanth, Ryan T. Johnson, Dr. Donna S. Amenta and Dr. John W. Gilje
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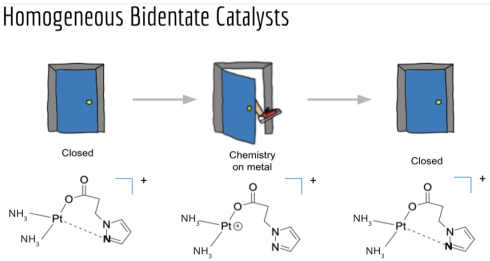
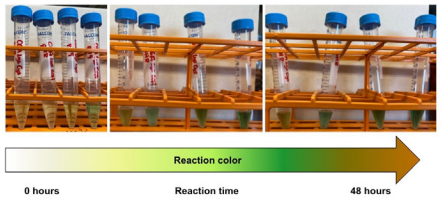


The reaction of 3,5-dimethyl pyrazole and methyl acrylate produced a N-pyrazolylpropanoate derivative (L1) by a base catalyzed Michael addition. Another N-pyrazolylpropanoate derivative (L2) was similarly synthesized from pyrazole and methyl acrylate. Saponification of L1 and L2 gave corresponding carboxylate salts. Acidification yields the corresponding carboxylic acids. Reactions of L1 and L2 with $(COD)PdCl_2$ formed $Cl_2Pd(L_n)2$. These were characterized by IR, NMR spectroscopy, elemental analysis and X-Ray crystallography. In both cases, the crystal structures are of the trans isomer with L2 is stable in solution but with L1, a trans/cis isomerization is observed.

Monitoring compounds involved with CGA-Lys greening in alkaline reaction mixtures

Andrew M. Roberts, Lynnea Gedney and Dr. Christine Hughey
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Chlorogenic acid (CGA), a polyphenol, reacts with amino acids at high pH (>8) to produce a green color that is undesirable in food products (e.g., baked goods). Our collaborators at Chapman University made this observation when cookies baked with sunflower butter, which is rich in CGA, turned green. At high pH, CGA oxidizes to its highly reactive, electrophilic quinone form. Amino acids with free primary amino groups, such as lysine, react with oxidized CGA to form a trihydroxy benzacridine (TBA) compound that is responsible for the green color. Introduction of thiols, such as cysteine (Cys) and glutathione (GSH) inhibit the greening reaction. This inhibition was monitored over 48 hours at pH 8 and 9 for CGA-Lys-Cys and CGA-Lys-GSH reaction systems. In addition to reactants, the oxidized dimers of Cys and GSH (or cystine and glutathione disulfide, GSSG) were monitored. The hypothesized green compound (TBA) was not observed, likely because the LC mobile phase is acidic, and it exists at high pH. The abundance of reaction species was measured by positive ion ESI q-TOF MS using both HILIC and reverse phase (RP) columns. HILIC offered better separation of the analytes than RP, therefore, trends reported here are from HILIC data. In the CGA-Lys-Cys reaction system, CGA was not detected after 20 hours at both pH 8 and 9. At 20 hours the concentration of Lys leveled off. Cys was not detected after 4 hours, which coincided with the greatest abundance of the oxidized product, cystine. After 4 hours, the cystine concentration decreased, then leveled off at 20 hours. Reactant concentrations were lowest and product concentrations highest at pH 9, as predicted. Similar results were observed in the CGA-Lys-GSH reaction system. However, GSH was not detected after 2 hours at pH 9 and 4 hours at pH 8. GSSG was not observed, likely because it eluted after the LC run ended. Therefore, further LC optimization is needed before the experiment is repeated. Visual observation revealed that Cys was more effective in hindering greening than GSH, which is contrary to Chapman's results. Future work will focus on optimizing the HILIC LC separation and mining the current data for other reaction products, in hopes that the reaction mechanisms involved can be elucidated.

Surface Morphology Evolution of $(MgNiCoCuZnCr)_{0.167}O$ Thin-Films

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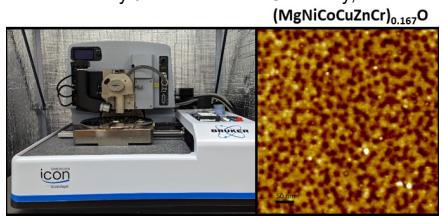

High entropy alloys (HEA) are alloys made of five or more metals. HEAs are of significant interest in materials particularly for refractory and structural applications. The premise of HEAs is that high configurational entropy tends to result in significantly fewer phases than otherwise predicted by the Gibbs Phase Rule through the formation of single-phase solid solutions. Entropy stabilized oxides (ESO), which are inspired by HEAs, are ceramics that contain five or more equimolar cations bonded to oxygen. Previous work with ESOs focused on the confirmation that entropy is the dominate thermodynamic component. This entropic reliance drives a solid-state transformation between a multiphase and single-phase state. In this work, I explore a fundamental study of the surface morphology of $(MgNiCoCuZnCr)_{0.167}O$ thin films using atomic force microscopy (AFM). Thin films synthesized were studied to determine if the nanoscale surface structure was impacted by the deposition conditions, i.e. background gas ratio, or deposition temperature, or if the overall ionic character of ceramics dictated the structure. The stability of the oxides were also tested by annealing the samples with a hydrogen flame. The stability was measured by observing the presence or lack of change in the structure, using powder X-ray diffraction (PXRD) and AFM.

Rational Design of Ultrafast PpcA-Ru(bpy)$_3$ Complexes

Zachary D. Ryan and Dr. Oleksandr Kokhan
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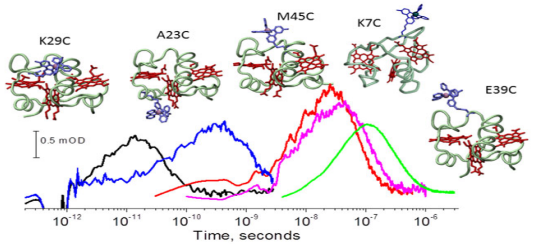

Converting light energy into its electrochemical equivalent requires precise control and fine-tuning of relevant kinetic and thermodynamic parameters of electron transfer (ET) steps. A particularly big challenge for artificial photosynthesis is to create the primary charge separation on the ultrafast (sub-nanosecond) time scale, as slower reactions are likely to require precious metal photosensitizers and produce significant amounts of reactive oxygen species. However, the structural requirements for ultrafast ET are poorly understood. The previous work from our lab has demonstrated that ET rates do not strictly depend on the distances. Similarly, we have demonstrated that short ET pathways through covalent bonds do not always result in ultrafast ET.Â Â We hypothesize that a rigid attachment of photosensitizers and efficient heat dissipation into the protein framework are needed for ultrafast ET. To test this hypothesis, we developed 13 new mutant forms of PpcA with the attachment cysteine sites showing restricted solvent exposure. We successfully labeled 11 out of 13 with Ru(bpy)$_3$ and observed the expected complex masses in LC-MS. Analytical size-exclusion chromatography revealed the absence of aggregation and predominantly monomeric forms. Temperature-dependent circular dichroism (CD) spectroscopy showed the absence of any significant destabilization of the protein structure due to mutations and photosensitizer attachment, apart from I38CRu. Finally, we measured electron transfer rates that show that 9 out of 11 PpcA-Ru(bpy)$_3$ complexes show ultra-fast electron transfer.

Statistical Analyses of Hemp and Hemp Product Cannabinoid Test Results

Rachel J. Stegmeier, Samantha Forbes, and Dr. Daniel Downey
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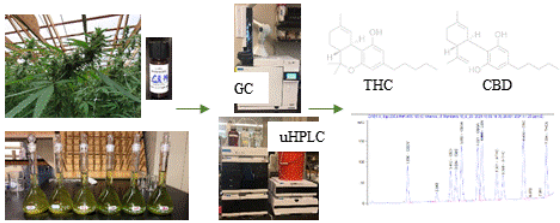
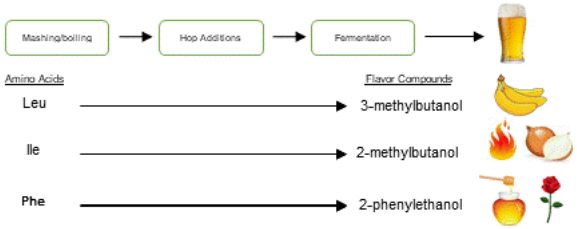


Cannabis sativa (hemp) is a flowering plant used for recreational and industrial purposes that contains a class of compounds called phytocannabinoids. Industrial hemp is a class of Cannabis sativa that has been propagated for low tetrahydrocannabinol (THC) and high cannabidiol (CBD) content. For legality, crops must be destroyed if THC content levels exceed the maximum legal limit of 0.30%. Regulators collect hemp samples from farms for testing at certified laboratories to ensure compliance. In the present study we have statistically evaluated all steps of the procedure including sample collection, handling, transport, drying, extraction, and instrumental analyses. We began by analyzing certified standards, limits of detection (LOD), limits of quantitation (LOQ), High-Pressure Liquid Chromatography Ultraviolet Detection (HPLC-UV) and Gas Chromatography Flame Ionization Detection (GC-FID). We also studied variations in cannabinoid content within different parts of the same plant and as well as compared to other crops. The handling and age of samples, degradation of calibration standards, extraction solvents, and other factors were also studied. Measured LOD / LOQ values were: total CBD ppm 0.33 / 1.39 (GC), 0.14 / 0.52 (HPLC); total THC ppm 0.13 / 0.48 (GC), 0.14 / 0.53 (HPLC). Data obtained by the standard methods showed that THC concentrations varied greatly from the top to the bottom of the plant with values of 0.39%, 0.25%, and 0.23% for THC, respectively. This indicates that overall cannabinoid content is not often represented in compliance testing, which may cause crops to be destroyed by regulators, resulting in a significant economic loss to farmers.

Evolution of Metabolites in a Single Malt, Single Hop (SMaSH) Beer Using Targeted and Untargeted Analysis

Leighann R. Weber[1], Amanda Cicali[1], Lynn E. Marsh[1], Steven Harper[1], Dr. Samuel A. Morton[2], and Dr. Christine A. Hughey[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA
[2]Madison Academic Brewery, Dept of Engineering, James Madison University, Harrisonburg, VA



Beer is a complex mixture with a unique flavor profile that is determined by the selection of malt, hops and yeast used. The advancement of MS-based metabolic techniques, affords the ability to profile both the volatile and nonvolatile compounds throughout the brewing process so that the development of flavor compounds from malt, hops and fermentation can be better understood. Here we look at the evolution of compounds in a single malt, single hop (SMaSH) pale ale. LC/MS and GC/MS were used to identify and track metabolites in biochemical pathways, such as the Erlich and phenylalanine degradation pathways, that are responsible for the production of flavor compounds. Through the analysis of samples collected throughout the brewing process, we observed a decrease in amino acid precursors (e.g., valine, leucine and isoleucine) and a subsequent increase in flavor compounds, specifically the fusel alcohols 3-methyl-1-butanol and 2-methyl-1-butanol. This increase was observed approximately 12 hours after the yeast was pitched and reached a steady state at ~70-100 hours. We are currently mining the data for intermediate metabolites involved in these pathways and have tentatively identified 3-phenyllactic acid, leucic acid, and phenylpyruvic acid. Future work will involve confirmation of these identification with authentic standards and their subsequent quantification.

Boronic Acid Orientation Effects on Hybrid Peptide-Polymer Properties

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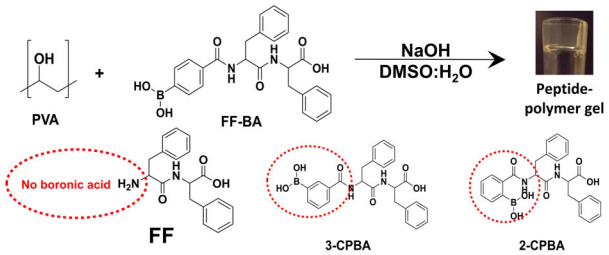

Peptides, particularly diphenylalanine, are known to self-assemble and form fibrous, supramolecular gels. Because these systems are biocompatible and non-toxic, they are useful for a number of different biomedical applications, such as tissue engineering and drug delivery. Despite these attractive features, optimizing the gelation conditions for peptide gelators is not trivial. Thus, there is an interest in developing methods that improve and simplify peptide gelation. In this work, we report a hybrid peptide-polymer gel formed under basic conditions with diphenylalanineboronic acid (FF-BA) and polyvinyl alcohol (PVA) in DMSO:H_2O mixtures. FF-BA was readily synthesized via solid-phase peptide synthesis, while PVA is commercially available. Gelation with this system occurs at ≥65% DMSO and requires excess NaOH, suggesting a boronate ester is a key structural feature of the gel network. Notably, in the absence of FF-BA, stiff gels are not observed. We propose that gelation occurs via the formation of boronate ester linkages between PVA and FF-BA and subsequent self-assembly of the peptide unit. The orientation of the boronic acid on the gelator were changed to ortho and para positions to observe effects on synthesis, gelation, and rheological properties.

2022 Department of Chemistry and Biochemistry Student Award Winners

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R.D. Cool Award	Connor J. Pearson
J.W. Chappell Scholarship (May 2021)	Rachel J. Stegmeier
Palocsay Award in Undergraduate Research	Stuart A. Regitz
Service Awards	Rachel E. Walsh
	Roujon A. Nowzari
J. W. Chappell Award	Tashi M. Poe
American Institute of Chemists	Lei R. Weber
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ACS Award	Olivia C. Mumma
Casali Scholarship (May 2021)	John M. Brymer
Dean's Award (Chemistry)	Ashleigh E. Outhous
Dean's Award (Biophysical Chemistry)	Trinity Perry
CRC First Year Student Award	Angelina V. Lo Presti
Outstanding Student Researcher Award	*to be announced*

Divisional Awards

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ACS Analytical Award	Rachel Steigmeier
ACS Environmental Award	Stephan G. Michaelov
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ACS Organic Award	Ani N. Davis
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