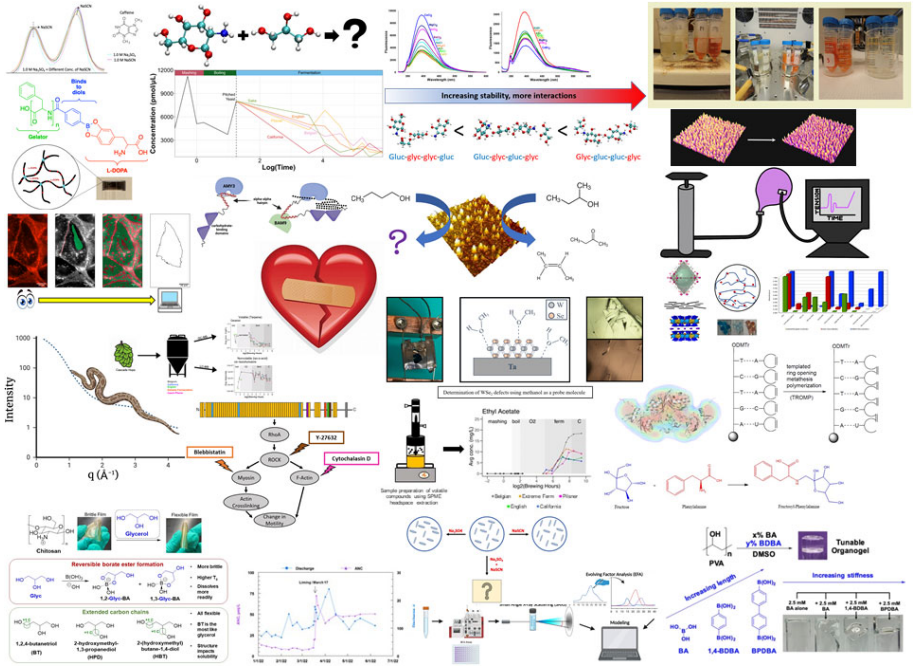
JAMES MADISON UNIVERSITY®

DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY



47TH ANNUAL SPRING UNDERGRADUATE RESEARCH SYMPOSIUM

THURSDAY APRIL 20, 2023

ORAL SESSION I: 9:15 – 11:00 AM (KING 259)

ORAL SESSION II: 1:00 – 2:15 PM (KING 259)

FRIDAY APRIL 21, 2023

POSTER SESSION: 1:00 – 3:00 PM (PCB LOBBY)

SPECIAL ANNOUNCEMENTS: 3:30PM (KING 159)

KEYNOTE ADDRESS: 3:35 – 4:35 PM (KING 159)

47th Annual Department of Chemistry and Biochemistry
Spring Undergraduate Research Symposium

Keynote Speaker

Kevin Bennett, PhD
(JMU Class of 1994)
Department of Chemistry & Physics
Hood College
Frederick, MD

Kevin Bennett is Professor in the Department of Chemistry and Physics at Hood College in Frederick, Maryland. He received his Bachelor of Science Degree in Chemistry with a minor in Economics at James Madison University in 1994. While at James Madison, he completed research in the area of acid rain impacts on stream water chemistry under the direction of Dr. Daniel M. Downey. Kevin received his Ph.D. in Analytical Chemistry from the University of Tennessee – Knoxville in 2000. While at Tennessee, he worked in the area of industrial process monitoring and electrospray mass spectrometry under the direction of Dr. Kelsey D. Cook. During his time at Tennessee, Kevin was fortunate to be an adjunct instructor at a small private liberal arts college. It took one semester of interaction with students in the research laboratory and classroom to make him realize that he wanted to become a full-time professor.

Kevin joined the faculty at Hood College in the fall of 2000. His research at Hood has been in the broad areas of Mass Spectrometry and portable x-Ray spectroscopy. The development of new ways of studying the fundamentals of electrospray ionization mass spectrometry is one area of his research interest. Improving knowledge of electrospray ionization is important to researchers in a range of fields including biology, biochemistry, chemistry, and geology. His other area of research interest is in the study of fundamental factors influencing spectra from portable x-ray spectroscopy instruments.

Kevin is currently the Principal Investigator on an interdisciplinary National Science Foundation Scholarship in Science, Technology, Engineering, and Mathematics (S-STEM) grant that attracts and supports academically talented low-income students in STEM during their undergraduate studies.

In his free time, Kevin enjoys outdoor activities, playing hockey, and running.

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
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 20, 2023 *(King 259)*		
9:15 am	Nina A. Metzger and Dr. Yanjie Zhang	Specific Ion Effects: Hofmeister Cations and Coumarin Fluorescence
9:30 am	Abigail E. Sholes and Dr. Christopher E. Berndsen	"What RcoM Sees:" Investigating Potential Binding Domains for the DNA Complex of the Px-RcoM-1 Transcription Factor
9:45 am	Quinn C. Harkrider, Stephanie Ouderkirk, Mason Ong, Dr. Callie Miller, and Dr. Nathan Wright	Investigating the Effect of Cell Architecture on Obscurin
10:00 am	*break*	
10:15 am	Stephanie N. Ouderkirk, Alex Sedley, Dr. Callie J. Miller, and Dr. Nathan T. Wright	Developing an Image Analysis Software Pipeline to Measure Cellular Mechanics
10:30 am	Zachary D. Ryan and Dr. Oleksandr Kokhan	An Affordable 3D-Printed UV Spectrophotometer
10:45 am	Roujon A. Nowzari, Clay P. Page, Isabel M. Romov, Dr. Nathan T. Wright	Bandaids on Broken Hearts: Preventing Protease-Mediated Degredation of Demsoplakin with Small Molecules

Oral Session II: Thursday April 20, 2023 *(King 259)*		
1:00 pm	Gabriella Newsome, Cindy Liu, and Dr. Isaiah Sumner	Analyzing the Interactions between Glucosamine and Glycerol
1:15 pm	Shyleigh A. Good and Dr. Daniel M. Downey	Water Chemistry of the St. Mary's River, Virginia: Liming to Mitigate Acid Rain
1:30 pm	Christine N. Buchholz, Ruby Adkins, and Dr. Christopher E. Berndsen	Rapid Analysis of Small Angle X-ray Scattering Data in Python
1:45 pm	Amanda R. Cicali, Eliana M. Diaz-Aceituno, Dr. Samuel A. Morton, Dr. Steven Harper, and Dr. Chrisi A. Hughey	Comparison of the amino acid metabolism of genetically different brewing yeasts
2:00 pm	Eric J. Shepard, Max B. Kelly, and Dr. Debra L. Mohler	Overcoming Degradation: A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs

(Student presenters underlined)

Poster Session: Friday April 21, 2023, 1:00 – 3:00 pm *(PCB lobby)*	
Heidi J. Arenas, Dr. Yanjie Zhang, Dr. Gina MacDonald	Effects of combined chaotropic and kosmotropic anions on caffeine aggregation using ATR-FTIR
Shannon E. Beck and Dr. Daniel M. Downey	Analytical Results of Cannabinoid-infused Gummy Candies for CBD and THC
Madeleine Benes, Roujon Nowzari, and Dr. Nathan Wright	Purification and in silico Modeling of ACM-linked Desmoplakin Mutants
Brooke M. Biltonen, Isaac Peregoy and Dr. Gretchen M. Peters	Peptide-boronic acid hydrogels for drug delivery applications
Xander M. Dirom, Ani Davis, Dr. Gretchen M. Peters	Stiffening PVA-BA gels by changing diboronic acid length
Logan C. Ealley, Dr. Brycelyn Boardman, Dr. Gretchen M. Peters	Impact of Plasticizer Structure in Chitosan Bioplastics
Haley Frankovich, Lyssa A. Garber, Ava J. Galgano, Erin Schell, John Yoo, Clayton Rogers, Jona Carmany, Charles L. Grant, Dr. Ashleigh E. Baber	Reactivity of Primary and Secondary Butanol Isomers on TiO_2/Au(111)
Ava J. Galgano, Erin D. Schell, Haley E. Frankovich, Jona P. Carmany, Charles L. Grant, John K. Yoo, Jacob L. St. Martin, Dr. Petra Reinke, and Dr. Ashleigh E. Baber	Effect of Thermal Annealing on WSe_2 Adsorption Sites
Juan M. Garcia, and Dr. Christine Hughey	Evolution of volatile and nonvolatile hop compounds throughout boiling and fermentation with genetically different yeast
Lynnea S. Gedney, Anna M. Moninger, Owen J. Tompkins and Dr. Barbara A. Reisner	Embedding Metal Organic Frameworks in Sodium Alginate/ Polyacrylic Acid Beads for Water Remediation
Angela J. Kayll, Jonathan Monroe, and Dr. Christopher E. Berndsen	X-ray Scattering of Carbohydrate Chains in Solution
Luke A. Langbo, Dr. Yanjie Zhang	^{13}C and ^{1}H NMR Studies of Combined Anion Effects on Caffeine Aggregation
Cindy Liu and Dr. Isaiah Sumner	Molecular Modelling of Biodegradable Plastics
Angelina V. Lo Presti, Amanda R. Cicali, Lynn E. Marsh, Leighann R. Weber, Christine A. Hughey, Steven Harper, and Dr. Samuel A. Morton	Identification of Amadori Products in a Single Malt, Single Hop (SMaSH) Beer
Stuart A. Regitz, Daniel P. Musikanth, Ryan T. Johnson, Dr. Donna S. Amenta, Dr. John W. Gilje	Synthesis of N-Pyrazolylpropanoate Derivatives as Potential Ligands with Palladium
Andrew M. P. Roberts, Eliana M. Diaz-Aceituno, Juan M. Garcia, Angelina V. Lo Presti, Kayla Moore, Viridiana Tirado, Dr. Steven Harper, Dr. Samuel A. Morton, and Dr. Christine A. Hughey	Evolution of Volatile Flavor Compounds Produced During the Fermentation of Beer with Genetically Different Yeasts
Angelina M. Sardelli, Dr. Christopher E. Berndsen, Dr. Jonathan D. Monroe, and Karen Siddoway	Structural Modeling and Analysis of β-amylase 9
Erin D. Schell, John K. Yoo, Haley E. Frankovich, and Dr. Ashleigh E. Baber	Morphological Studies of TiO_2 Nanoparticles on Au(111)
Kamrin D. Shultz, Quinn C. Harkrider, Stephanie N. Ouderkirk, Dr. Nathan T. Wright, and Dr. Kristopher Kubow	Quantifying cellular mechanics using time-lapse fluorescent microscopy

(Student presenters underlined)

Special Announcements: Friday April 21, 2023 *(King 159)*	
3:30pm	Announcement of Chemistry and Biochemistry Student Award Winners

Keynote Address: Friday April 21, 2023 *(King 159)*		
3:35 - 4:35 pm	Kevin Bennett, PhD JMU Class of 1994	Cations versus Anions – The Importance of Keeping Positive during Scientific Research

Keynote Address

Friday, April 21, 2023 at 3:35 pm
King 159

Cations versus Anions – The Importance of Keeping Positive during Scientific Research

Kevin Bennett, PhD
(JMU Class of 1994)
Department of Chemistry & Physics
Hood College
Frederick, MD

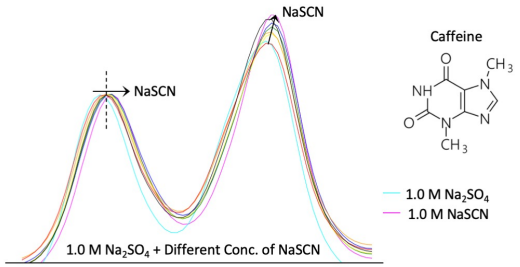
Mass spectrometry can provide a wide range of information on compounds that produce either positive or negative ions upon electrospray ionization (ESI). Improving knowledge of electrospray ionization is important to researchers in a range of fields including biology, biochemistry, chemistry, and geology. Finding ideal ionization conditions for analytes is important to maximize data quality. This talk will center on the study of a range of target compounds and the impact of ESI conditions on the observed data quality. For negative ion mode, this research focused on the analysis of the analytes Cocaine, Naproxen and Ibuprofen. Optimal ionization conditions were determined over a wide range of solution and instrumental conditions. For positive ion mode, the research focus was on the analysis of polyethylene glycol (PEG) and polypropylene glycol (PPG) target analytes. Solutions of each polymer were studied with different complexing cations (Li^+, Na^+, K^+, Rb^+, Cs^+, NH_4^+ and Ag^+).

STUDENT ABSTRACTS

(Student presenters underlined)

Effects of combined chaotropic and kosmotropic anions on caffeine aggregation using ATR-FTIR

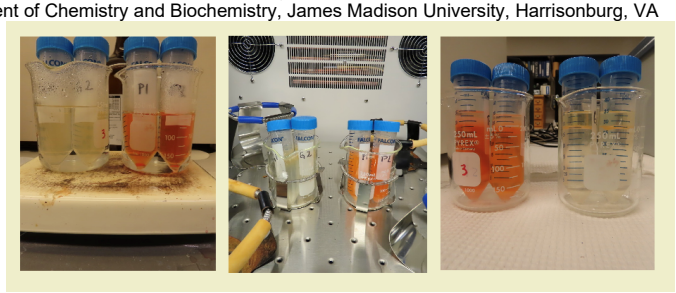
Heidi J. Arenas, Yanjie Zhang and Dr. Gina MacDonald
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



The Hofmeister series ranks ions based on their stabilizing effects. Ion's ability to destabilize (salting-in) and stabilize (salting-out) proteins. It is important to understand the behavior of ions in aqueous solutions. In this study, caffeine was used as a model compound to study mixed ion interactions with solute molecules. We studied the combined effects of different kosmotropic and chaotropic salts on caffeine vibrations in both deuterium oxide (D_2O) and water (H_2O) using attenuated total reflection-fourier-transform infrared (ATR-FTIR). Different concentrations of salts were studied to determine the relative influence of each ion on caffeine aggregation. Our results show that NaSCN and $NaClO_4$ shift the vibrations at ~1650 and ~1700 cm^{-1} to lower wavenumbers indicating less aggregation and increased solvation. The addition of Na_2SO_4 results in shifts to higher wavenumbers indicating increased aggregation and decreased solvation. Infrared studies of caffeine in a combination of salts show that the effects of NaSCN and $NaClO_4$ dominate over the influence of Na_2SO_4. The mixture of two chaotropic ions shows an additive function.

Analytical Results of Cannabinoid-infused Gummy Candies for CBD and THC

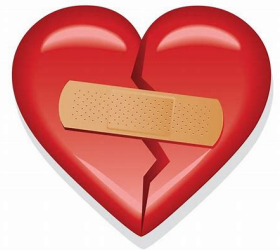
Shannon E. Beck and Dr. Daniel M. Downey
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Cannabis sativa is an annual plant that produces phytocannabinoids that have alleged medical benefits. A variety of dietary supplement products containing varying amounts of cannabidiol (CBD), tetrahydrocannbinol (THC), and other cannabinoids extracted from cannabis plants are now available. Product labels indicate mass levels per dose of these cannabinoids. We have been analyzing various gummy candy products to determine if manufacturer claims are reliable. State compliance testing is required for products marketed in dispensaries, but is not enforced for products sold in non-dispensary storefronts. One of the most common dietary supplement product types with cannabinoids are gummy candies. Gummies are made by combining gelatin, pectin, sugars, flavoring, and dyes with extracts from hemp or marijuana plants. Analysis of the gummies follows the state-compliance testing method for products sold in dispensaries. Analytical steps include dissolution in water and extraction by salting with acetonitrile. Ultimately, Ultra High-Performance Liquid Chromatography-Ultraviolet Detection (UHPLC-UV) calibrated with an eleven-component standard was used for analyses. Results to date indicate that there is considerable difference between market claims and actual cannabinoid amounts in many gummy products sold outside of dispensaries.

Purification and in silico Modeling of ACM-linked Desmoplakin Mutants

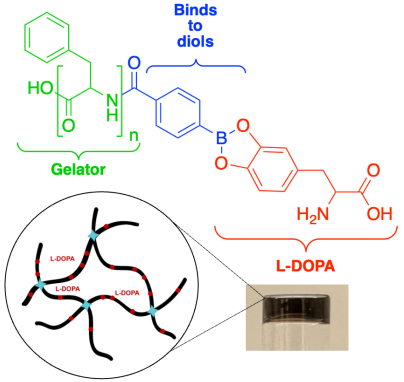
Madeleine Benes, Roujon Nowzari, and Dr. Nathan Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Desmoplakin (DSP) is an integral component of the desmosome, a subcellular structure, that links the intermediate filament networks of adjacent myocytes. In cardiomyocytes, the desmosome maintains both cell-to-cell adhesion and promotes electrical synchronization. Some DSP mutants are hypersensitive to calpain cleavage, which results, eventually, in clinical arrhythmogenic cardiomyopathy. We want to find small molecules that inhibit this hypersensitive phenotype. Here, we describe the process of growing and purifying one of these hypersensitive mutants, S442F. Once this is accomplished, we will test a bevy of small molecule candidates for their ability to decrease calpain cleavage in both experimental and computational settings.

Peptide-boronic acid hydrogels for drug delivery applications

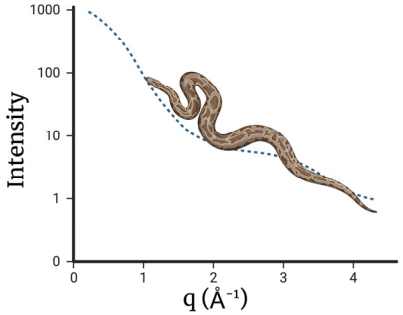
Brooke M. Biltonen, Isaac Peregoy, and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Supramolecular gels are a growing area of interest in the biomedical world due to their biocompatibility, their propensity for manipulation, and their ability to uptake and release drugs in a controlled fashion. Levodopa (L-DOPA) is a Parkinson's drug that is enzymatically decarboxylated to produce dopamine in the brain. However, because L-DOPA is taken orally, it rapidly degrades in the gastrointestinal tract and leads to patient discomfort and diminished efficacy. Incorporation of L-DOPA into gel media has been shown to improve patients' responses. However, there remains a lack of control over the drug's release in these systems. Here, we report a supramolecular peptide-boronic acid gelator capable of incorporating and releasing L-DOPA via reversible boronate ester formation. A small library of peptide-boronic acids were synthesized via solid-phase peptide synthesis (SPPS). We found that self-supporting hydrogels formed with the triphenylalanine-boronic acid conjugate (FFF-BA) at greater than 8 mM at neutral pH. Using a combination of NMR titrations, diffusion ordered spectroscopy (DOSY), and alizarin red S fluorescence assays, we determined that the L-DOPA reversibly binds to FFF-BA via boronate ester formation both in solution and in the gel network. Additionally, the triggered release of L-DOPA was investigated. This material has been fully characterized and has potential as an L-DOPA delivery system.

Rapid Analysis of Small Angle X-ray Scattering Data in Python

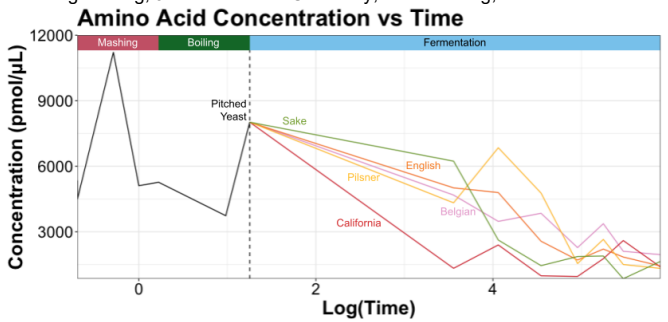
Christine N Buchholz, Ruby Adkins, and Dr. Christopher E. Berndsen
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Everyone who has taken a Biochemistry class has heard the phrase structure determines function. Small-angle X-ray Scattering (SAXS) is a method that measures the angle of scattering from a sample to gain data on the structural information. SAXS data can be collected in a variety of ways including high-throughput SAXS which may have applications for drug discovery and studies of biomolecules. Users currently receive un-analyzed data and they need to manually work through to analyze data and determine if radiation damage is present, which takes time and expertise. Because the beamline collects replicates on the same sample, the user needs to know if the samples were damaged by the X-ray beam as replicates were collected. An automated system could help scientists know where to preliminarily focus their efforts. We are writing software to analyze high-throughput SAXS data in collaboration with the SYBILS Beamline which will guide the user in their analysis. We have written a program using Python, called “Rgifier”, that analyzes the data and calculates standard values that determine size and shape along with the error of these calculations. The software writes the results into a summary .csv file that has the values of interest from the Porod and Guinier regions. We have tested the code on standard data sets from the SASBDB database and experimental data sets. The code is sensitive enough to detect radiation damage across frames in datasets. We analyzed protein and non-protein biomolecules in Rgifier and compared it to manual fitting to determine accuracy. The Rgifier is accurate for different types of biomolecules. We are preparing the Rgifier for integration into the Beamline workflow. Our preliminary code will enhance the rate at which scientists can describe the breadth of biomolecule structure and lead to a greater ability to address the problems of the future.

Comparison of the amino acid metabolism of genetically different brewing yeasts

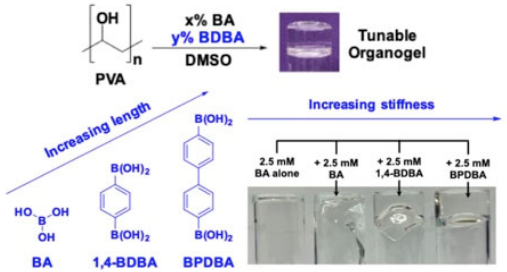
Amanda R. Cicali[1], Eliana M. Diaz-Aceituno[1], Samuel A. Morton[2], Steven Harper[2], and Dr. Chrisi A. Hughey[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA
[2]Department of Engineering, James Madison University, Harrisonburg, VA



The selection of malt, hops, and yeast affects the quality and flavor of the final beer. Here a pale ale was brewed with a 2-row Briess malt and Cascade hops. The wort was transferred to five fermentation tanks and fermented with the following genetically different yeast: Belgian Saison, California ale, Czech pilsner lager, English ale, and Extreme fermentation. The aim of the work was to monitor amino acid metabolism during fermentation. Amino acids are extracted from the malt during mashing and utilized by the yeast to produce flavor compounds in various biochemical pathways, such as the Ehrlich pathway. In this pathway, amino acids are converted to a keto-acid via transamination. Decarboxylation, reduction, and oxidation follow to produce an aldehyde, alcohol, and ester, respectively. To monitor this pathway throughout fermentation, hydrophilic interaction liquid chromatography-mass spectrometry (HILIC-MS) was used to quantify amino acids. Reverse-phase (RP) LC-MS, using negative ion electrospray (ESI) mode, was collected to increase the likelihood of observing pathway intermediates. SPME Arrow and gas chromatography-mass spectrometry (GC-MS) data was collected to quantify the aldehydes, alcohols, esters, and other flavor compounds. For each yeast, it can be shown that the amino acid concentration is highest halfway through mashing and decreases as fermentation progresses. To date, efforts to identify pathway intermediates have focused on reactions that produce methyl butanols and phenyl ethyl alcohol–the most abundant volatile compounds produced during fermentation, excluding ethanol. The keto-acids that form from leucine/isoleucine in the Ehrlich pathway have been putatively identified but need confirmation with standards. The subsequent aldehydes and alcohols were quantified by GC/MS. Phenylalanine yields phenyl ethyl alcohol. The identity of the intermediate phenylpyruvate was confirmed. Phenylacetaldehyde was identified and phenylethyl alcohol was quantified in GC/MS data. Future work will focus on confirming these intermediates with purchased standards.

Stiffening PVA-BA gels by changing diboronic acid length

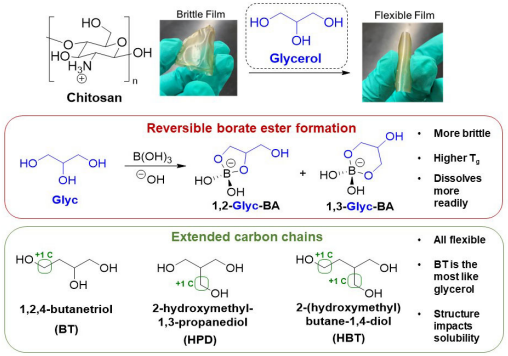
Xander M. Dirom, Ani Davis, and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Gels are versatile materials that have numerous practical applications such as environmental waste management, cosmetic items, drug delivery, and biomedical products. Because these applications require different material properties, there is an interest in developing gels that can be easily manipulated. In our previous work, we found that adding a diboronic acid crosslinker to a polyvinyl alcohol (PVA) – boric acid (BA) organogel yielded a tunable material. While BA alone formed viscous dispersions with PVA in DMSO, substituting small amounts of BA for 1,4-benzenediboronic acid (1,4-BDBA) dramatically improved the material properties and gelation. We theorized that by crosslinking PVA itself, 1,4-BDBA improved BA's ability to form crosslinks and gel PVA. Here, we investigated the impact of the crosslinker's length on BA crosslinking within PVA organogels. Specifically, we compared PVA gels formed with BA alone to those made with mixtures of BA and 1,4-BDBA or BA and 4,4'-biphenyldiboronic acid (BPDBA). Notably, we found that the addition of BPDBA improved the properies of the PVA-BA gel in a similar fashion to 1,4-BDBA, but yielded even stiffer gels. The influence of length and flexibility is further being investigated using a series of aryl diboronic acids (n-BEDBA) that we have designed. These compounds are comprised of two phenyl boronic acid units with a linker of varying length. We theorize that the length of the crosslinker will directly impact the stiffness and stability of the PVA-BA gel and thus will allow us to easily manipulate the resulting material properties. 1-BEDBA has been synthesized to test an even longer crosslinker. 1-BEDBA will be tested in PVA organogels.

Impact of Plasticizer Structure in Chitosan Bioplastics

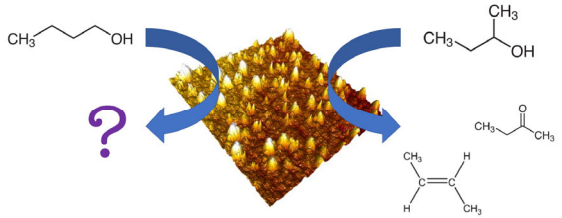
Logan C. Ealley, Dr. Brycelyn Boardman, and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA



Chitosan is a material used for bioplastics due to its ability to form a plastic film on its own. The films are quite brittle themselves, so a plasticizer known as glycerol was added to make the films more plastic like. Boric acid was incorporated into the films to see how it would affect the films. It made the films more brittle but allowed them to dissolve in water. Next carbon chains in between OH groups were changed by adding carbons. This showed to make the films a range of either brittle like chitosan itself or flexible like when glycerol was added. Since these films did not have boric acid, they did not dissolve as well in water. Rather than putting boric acid in the films which compromises the properties, the films were treated with aqueous boric acid. Differences were observed in film solubility in aqueous boric acid.

Reactivity of Primary and Secondary Butanol Isomers on TiO_2/Au(111)

Haley Frankovich[1], Lyssa A. Garber[1], Ava J. Galgano[1], Erin Schell[1], John Yoo[1], Clayton Rogers[1], Jona Carmany[2], Charles L. Grant[1], and Dr. Ashleigh E. Baber[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA
[2]Department of Physics and Astronomy, 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 which make it an attractive alternative fuel. Understanding the fundamental thermal catalysis processes of butanol over heterogeneous model catalysts can aid in the design of more efficient catalysts. Butanol isomers give rise to products including isobutyraldehyde, 2-butanone, butyraldehyde, isobutene, and butene, all of which have applications ranging from gasoline additives to bioplastics. For the partial oxidation of butanol isomers, TiO_2/Au(111) inverse model catalysts are promising due to their ability to catalyze redox reactions of C1 – C3 alcohols. Titania coverage effects were not reported for methanol or 2-propanol, but lower TiO_2 coverages in the presence of excess oxygen enhance selectivity of the partial oxidation of ethanol. To better understand how butanol breaks down in heterogeneous catalytic processes, temperature programmed desorption (TPD) is used to investigate its reaction. In this study, the reactivity of butanol isomers, specifically 1-butanol, 2-butanol, and isobutanol, on TiO_2/Au(111) was investigated. TPD was used to detect products and atomic force microscopy (AFM) highlighted the morphology of the surface. At low coverages of TiO_2, only 2-butanol showed expected oxidation reactivity, while, 1-BuOH exhibited low reactivity and formed reduced products, and isobutanol produced the recombinative product. At higher coverages of TiO_2/Au(111), 2-butanol formed both oxidized and reduced products, 1-butanol only formed reduced products, isobutanol produced oxidation, reduced, and recombinative products. The selectivity of the reaction was not altered during successive desorption experiments, indicating that the model catalyst was stable without reoxidation between experiments. AFM images show that the Au(111) crystal has ~0.13 ML and 0.27 ML of TiO_2 with predominantly 1D wire-like nanoparticles. Higher coverages of TiO_2 result in more particles distributed across the surface indicating that the reactivity was influenced by butanol proximity to TiO_2 nanoparticle rather than differences in size or shape.

Effect of Thermal Annealing on WSe_2 Adsorption Sites

Ava J. Galgano[1], Erin D. Schell[1], Haley E. Frankovich[1], Jona P. Carmany[1], Charles L. Grant[1], John K. Yoo[1], Jacob L. St. Martin[1], Dr. Petra Reinke[2] and Dr. Ashleigh E. Baber[1]
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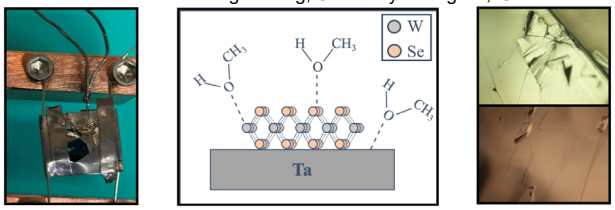

Determination of WSe_2 defects using methanol as a probe molecule

Transition metal dichalcogenides (TMD) are two dimensional (2D) materials gaining attention due to their unique properties at low dimensions. 2D TMDs have shown promise as catalysts for CO_2 hydrogenation and the hydrogen evolution reaction. Defects, or surface irregularities, of the atomic structure of 2D TMDs, are suggested active sites; however, the link between defects, electronic structure, and activity is unknown, which limits the ability to control reactivity. Prior to investigating the chemical reactivity of the 2D TMD, WSe_2, layers of the material were transferred from a bulk sample to a tantalum substrate via mechanical exfoliation. The WSe_2/Ta was gently annealed under ultrahigh vacuum (UHV) conditions at varying temperatures and times to increase the defect inventory. The results shown here will highlight the reactivity of methanol as a probe molecule using UHV temperature programmed desorption on WSe_2/Ta. In addition, optical and atomic force microscopy characterization will be used study surface defects. After annealing to 400 ºC for 30 min, the appearance of a new desorption feature for methanol was observed indicating a change of surface defect concentration. The combination of this data will lead to a better understanding of the correlation between the structure of materials and the molecular adsorption (sticking) and desorption (releasing). Future work will study the change in defect inventory by ion bombardment in comparison to the annealing procedure.

Evolution of volatile and nonvolatile hop compounds throughout boiling and fermentation with genetically different yeast

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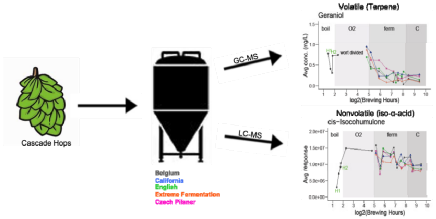

Hops are added to beer during brewing to impart flavor and to preserve the beer. Volatile terpenes impart hints on citrus, pine or medicinal flavors. While nonvolatile hop acids, like α-acids, impart bitterness. Here we monitor the evolution of volatile and nonvolatile hop-derived compounds in a pale ale throughout boiling and fermentation with five genetically different yeasts: Belgian Saison, California ale, Czech pilsner lager, English ale, and Extreme fermentation. Cascade hops were added at the beginning and end of the boil. Volatile hop-derived compounds were quantified by SPME GC/MS. The evolution of nonvolatile compounds was monitored by LC coupled to a triple quadrupole mass spectrometer (QqQ). Due to the lack of standards, compounds were putatively identified by matching MS/MS spectra to the literature and responses normalized against the first sample collected during boiling. Ten terpenes were identified and quantified. A ~85% decrease was observed for the most volatile terpenes between the first and the end of boiling. Concentrations were further decreased during fermentation. Statistical differences were observed across yeast strains for all terpenes except caryophyllene oxide. To facilitate analysis of the nonvolatile hop compounds, trends were reported for one compound within each compound class: α-acids, iso-α-acids, β-acids, humulinones, and prenylflavonoids. α-acids, β-acids and prenylflavonoids exhibited an increase after each hop addition. A steady increase throughout boiling was observed for isomerized and oxidized products of the α-acids, β-acids and prenylflavonoids. The concentration generally decreased for all compounds during fermentation. Statistical differences across yeast strains were observed for all compounds except the isomerized and oxidized products. A periodicity, likely due to the uptake/utilization by the yeast and subsequent release into solution was observed. Collectively, the GC/MS and LC/MS data gave a comprehensive look at the biotransformation of hop-derived compounds during beer fermentation.

Embedding Metal Organic Frameworks in Sodium Alginate/ Polyacrylic Acid Beads for Water Remediation

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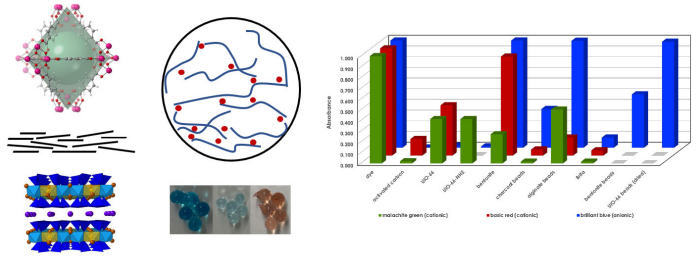

Porous materials can be used to adsorb contaminants from water. Currently, activated carbon and clays like bentonite are used as part of the water purification process. Metal organic frameworks (MOFs) are crystalline materials that are being explored for water purification. Research shows that changing the composition of the MOF alters the nature and amount of the contaminant that can be adsorbed. UV-Visible (UV-Vis) spectroscopy is used to quantify contaminant removal. However, MOFs typically crystallize as nanoparticles which become suspended in solution leading to inaccurate results due to light scattering. To prevent scattering from suspended nanoparticles, sodium alginate and polyacrylic acid (PAA) were used to immobilize the MOFs. Four MOFs (UiO-66, UiO66-NH2, ZIF-8, ZIF-67), bentonite, and activated carbon were embedded in sodium alginate / polyacrylic acid beads. The beads were characterized with powder x-ray diffraction (PXRD). The uptake of cationic methylene blue, anionic brilliant blue, and cationic basic red dyes were measured.

Water Chemistry of the St. Mary's River, Virginia: Liming to Mitigate Acid Rain

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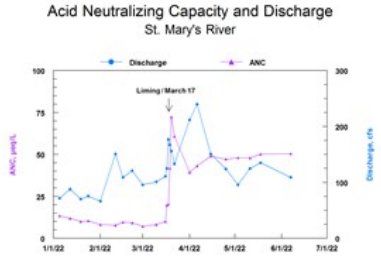

St. Mary's Wilderness is a federally designated portion of the George Washington National Forest in Augusta Co., Virginia. The 10,000-acre Wilderness is drained by the St. Mary's River with five major tributaries: Sugartree Branch, Mine Bank Creek, Bear Branch, Chimney Branch, Hogback Creek and a small tributary, Dawn's Branch that drains a wetland. The river and its tributaries experienced loss of aquatic life in the late 1990s due to acid rain. In 1999, 2005, 2013 and March 2022, limestone was introduced into all of the streams in the Wilderness to neutralize acidity. Dosage was ~200 tons evenly distributed to 7 in-stream sites. Water samples were collected at the Wilderness boundary and throughout the Wilderness upstream and downstream of the liming sites. The frequency of sample collection has varied throughout the period of the project. Analytical data for these samples has been used to judge the initial effectiveness of the limestone treatment and estimate longevity. Key water chemistry parameters for the weekly samples showed average increase in pH from pH 5.87 to pH 6.48, increase in ANC from 9.6 to 45.4 µeq/L, increase in Ca / H ratio from 25.7 to 184.7 and decrease in Al from 13 to 7 ppb. The upstream and downstream data pairs for each liming site also showed improvement in water quality. Longevity estimates indicate the Wilderness will not need another limestone treatment for at least 7 years. Due to the Clean Air Act and improved rainfall water quality, it is possible that no future treatment may be needed.

Investigating the Effect of Cell Architecture on Obscurin

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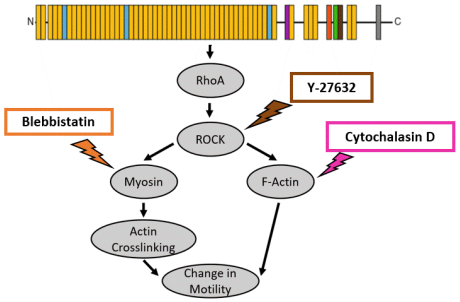

Obscurin is a large cytoskeletal protein found in epithelial and muscle cells. It is the second most mutated protein in breast and colorectal cancers and is significantly downregulated in pancreatic cancer. Obscurin activates ROCK via RhoA, which in turn activates myosin, stimulates F-actin polymerization, and modulates cellular motility and migration. Likewise, obscurin knockdown leads to an epithelial to mesenchymal transition (EMT), a hallmark of cancer progression. Previous work in our lab showed that MDCK cell expresses either no or very little endogenous obscurin. Here, we introduced a shortened obscruin construct, term obscA-tsMod, that contains a force sensitive FRET sensor. We find that in normal culture conditions, this construct is under >5pN of force, and that obscurin partially colocalizes at membrane areas that are also under tension. Chemically induced cytoskeleton perturbation correlates with obscA-tsMod being under less tension. Mechanically perturbing the whole cell by stretching and relaxing the cell membrane also correlates with obscA-tsMod being under in tension. However, obscurin presence has no effect on cell velocity, and disruption of upstream motility signaling through the rhoA pathway is not correlated with changes in obscA-tsmod tension. Together, this suggests that obscurin tension can be modulated, and is likely tied to cytoskeletal changes within MDCK cells.

X-ray Scattering of Carbohydrate Chains in Solution

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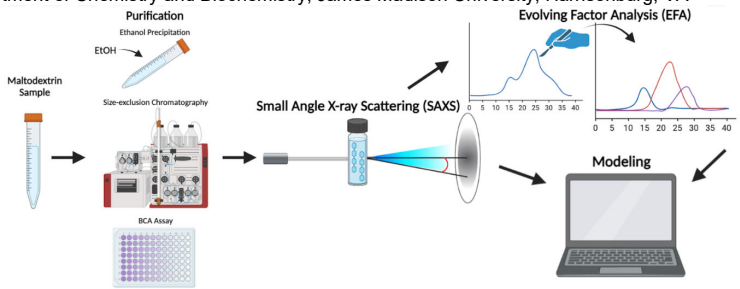

Starch is a form of long-term energy storage in plants and is one of the most widely used molecules by humans. Plants periodically degrade stored starch as fuel for metabolism and other metabolic processes. Animals, including humans, use starch as a source of nutritional energy and there are numerous industrial uses for this molecule. Currently there is limited information on how starch-degrading enzymes, including amylases, bind to and cleave starch. This project aims to describe the structure of the carbohydrate substrate of amylases, thus allowing us to better describe how amylases bind to and degrade starch. Knowing information about the structure of our substrate, maltodextrin, can lead to information about the functionality of amylases through activity assays, thus allowing us to further understand the function of amylases in humans and plants. The main techniques used to study starch structure were Small Angle X-Ray Scattering (SAXS) and in silico starch modeling. The initial results from our SAXS datasets revealed impurities in commercially acquired polysaccharides. We then purified maltodextrin samples using ethanol precipitation and size-exclusion chromatography to enrich the samples for the target carbohydrates. We then used Size Exclusion Chromatography coupled SAXS (SEC-SAXS) and High-Throughput SAXS (HT-SAXS) to assess the structure of purified maltodextrin chains in solution. The purification method that was created led to clearer SAXS results compared to previous unpurified maltodextrin SAXS datasets. We are further applying this purification pipeline to starch and model starch systems. We have also recently used Evolving Factor Analysis (EFA) to deconvolute overlapping peaks in SEC-SAXS data to try to aid in the fractionating of the sample. From our current and future work, we will describe and compare the substrate specificity of amylases leading to a better understanding of plant starch remodeling, which will aid in the development of new uses of starch for humans.

^{13}C and ^{1}H NMR Studies of Combined Anion Effects on Caffeine Aggregation

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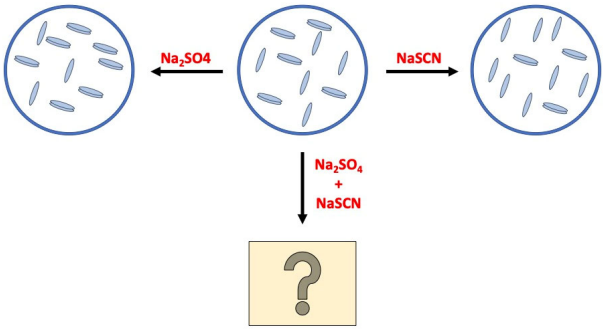

The Hofmeister series ranks ions' relative ability to influence various processes in aqueous solution such as protein solubility, protein folding, and polymer aggregation. This study aims to investigate the effects of combined anions from the Hofmeister series on caffeine aggregation using ^{13}C and ^{1}H NMR. The chemical shift of caffeine in the presence of Na_2SO_4, NaSCN, NaBr, NaH_2PO_4, NaI, and combinations of two of these salts are measured and compared to the chemical shift of caffeine in a salt-free solution. The conclusions of this research will be presented in this poster and discussion.

Molecular Modelling of Biodegradable Plastics

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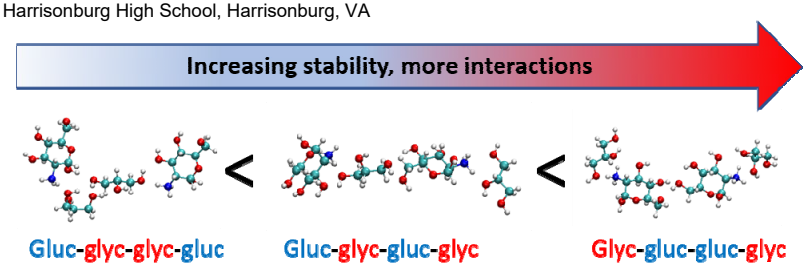

With millions of tons of plastic continuing to pile up, it is imperative that we find new, sustainable solutions. One way to do so is to use chitosan (which comes from shrimp shells) and glycerol (which is a commonly used additive and plasticizer) to form biodegradable plastics. However, the exact way that these molecules form polymers is unknown. Using a molecular modelling software that uses density functional theory (DFT), the aim is to find the most stable structures in which these molecules interact with each other. The advantage of modelling is that it allows for atomic-level resolution and the possibility of molecular-level manipulation. By running calculations, the lowest energy structures can be found, and conclusions can be drawn from patterns found in energy level in relation to molecular structure. The main focus was on the interactions between glucosamine (found in chitosan) and glycerol, and two main patterns emerged: the most stable structures had the greatest number of intermolecular interactions and were symmetric.

Identification of Amadori Products in a Single Malt, Single Hop (SMaSH) Beer

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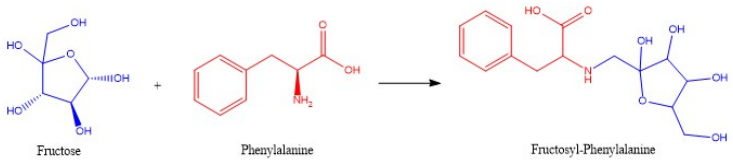

Amadori products are the first key intermediate of the Maillard reaction, a myriad of reactions between amino acids and reducing sugars that form flavor compounds and pigments. The Maillard reaction and its products are important for the final color and flavor of a beer. By monitoring the formation and evolution of Amadori products throughout the brewing process, a better understanding of the molecular-level interactions in beer can be gained, ultimately allowing brewers to manipulate flavor profiles.The Maillard reaction is initiated when a Schiff's base is formed between the carbonyl of the reducing sugar and an amino acid. Via Amadori rearrangement, this imine transforms into 1-amino-1-deoxyketoses. These products were observed by RP positive ion ESI q-TOF-MS in a single malt, single hop (SMaSH) beer produced in the Madison Academic Brewery. Specifically, fructosyl-phenylalanine (Fruc-Phe) and fructosyl-leucine/isoleucine (Fruc-Leu/Ile) were putatively identified by using their mass, low retention times, MS/MS fragment ions, and response profile during brewing. These compounds then undergo enolization and release of the amino acid to produce 1-deoxy-2,3-hexodiuloses (3-DG) or 3-deoxy-2-hexosuloses (3-GH). Because these compounds are not easily ionized by electrospray ionization without derivatization, they were not detected. Dehydration products of Amadori products were investigated, but only furfural, from the dehydration of a pentose Amadori product, was found in appreciable quantities and quantified. Amadori products also undergo Strecker degradation to produce Strecker aldehydes, volatile organic flavor compounds essential to a beer's flavor. The evolution of Strecker aldehydes was investigated and it was found that, while Strecker aldehydes form during mashing, they are later lost to volatilization during boiling. Future work will focus on quantifying and monitoring the precursor sugars to Amadori products so that a broader picture of the Maillard reaction in beer can be gained.

Specific Ion Effects: Hofmeister Cations and Coumarin Fluorescence

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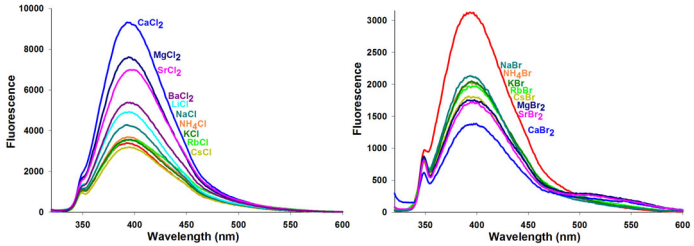

Fluorescence, or the emission of radiation due to excitation at a specific wavelength, was used to study the Hofmeister cation series' interactions in chlorine and bromine salts with coumarin in an aqueous solution. Coumarin was chosen as a model compound due to its hydrophobic and hydrophilic moieties allowing different ions to interact in contrasting ways. Coumarin was excited at 310 nm, and emission spectra of coumarin were measured from 320-600 nm in each experiment at differing salt concentrations for each cation. Hofmeister cations in chloride salts enhanced the fluorescence of coumarin, while cations in bromide salts decreased the fluorescence of coumarin. This information was used to further study the effects of mixed cations on coumarin fluorescence in an aqueous solution. These experiments indicated the additive nature or non-additive nature of cations depending on pairings. The quenching mechanisms of cations were investigated by using Stern-Volmer plots of chloride and bromide salts at 20°C and 50°C. The complete results of Hofmeister cations effects on coumarin fluorescence will be presented.

Analyzing the Interactions between Glucosamine and Glycerol

Gabriella Newsome[1], Cindy Liu[2] and Dr. Isaiah Sumner[1]
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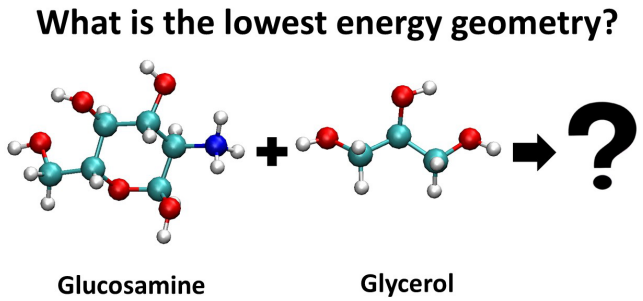

Creating new and efficient bioplastics will reduce how much waste is polluting the environment. A mixture of chitosan (glucosamine) from shrimp shells and a glycerol plasticizer can make a new environmentally friendly bioplastic. However, the molecular interactions between glucosamine and glycerol are not well understood. Therefore, we use computational chemistry to better understand the molecular interactions between the two. We employ a genetic algorithm in the OGOLEM software to calculate all possible low-energy structures formed between glucosamine and glycerol. Using a genetic algorithm helps ensure that we examined a wide variety of structures. Considering the genetic algorithm requires many calculations, a computationally inexpensive, semi-empirical method, PM7, was utilized for calculating the energies. These geometries were then sieved through DFT optimizations to increase the accuracy of the results. The structures are initially filtered with M06-2x/6-31+G(d). The final structures are calculated with M06-2x/6-311+G(2d,p). Different ratios of glucosamine and glycerol were used in this process and the lowest energy structures are compared to experimental results. Based on the data collected so far, the positive charge on the amine group in glucosamine is the dominant factor in all interactions.

Bandaids on Broken Hearts: Preventing Protease-Mediated Degredation of Demsoplakin with Small Molecules

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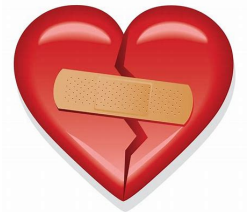

The desmosome is an intercellular protein complex crucial for cell-cell adhesion. Found in muscular and cutaneous tissue, the desmosome maintains tissue integrity under significant mechanical stress through the linking of cellular intermediate filament networks. Desmoplakin (DSP) is integral to the desmosome, and functions by connecting desmosomal cadherins to intermediate filaments. Multiple missense mutations in a DSP 'hotspot region' (residues 299–515) are causally linked to arrhythmogenic cardiomyopathy. Mutated DSP maintains structural integrity. However, mutations expose a normally-occluded calpain cleavage site (residues 447-451), resulting in decreased protein levels in affected tissues. Calpain is crucial for normal muscle development and maintenance. Therefore, instead of inhibiting calpain function, here we aim to find a "molecular band-aid" for DSP; a molecule that blocks this cleavage site without influencing calpain function. We have partially screened a library of FDA-approved drugs by monitoring fluorescence polarization of FITC-labeled DSP in the presence of protease. Molecules that prevent degradation are subjected to a secondary assay against FITC-BSA to screen for protease-specific inhibition. Molecules that specifically inhibit DSP degradation but not BSA degradation are then subjected to molecular dynamics-based drug docking studies. Preliminary data reveal that drug 'hits' tend to be larger organic molecules. Most, but not all, of these molecules stay bound to DSP over > 50 ns of simulation, and in addition have smaller calculated dissociation constants. Together, these preliminary data validate the feasibility of this workflow for identifying promising small molecules that prevent DSP degradation.

Developing an Image Analysis Software Pipeline to Measure Cellular Mechanics

Stephanie N. Ouderkirk[1], Alex Sedley[2], Callie J. Miller[3], and Dr. Nathan T. Wright[1]
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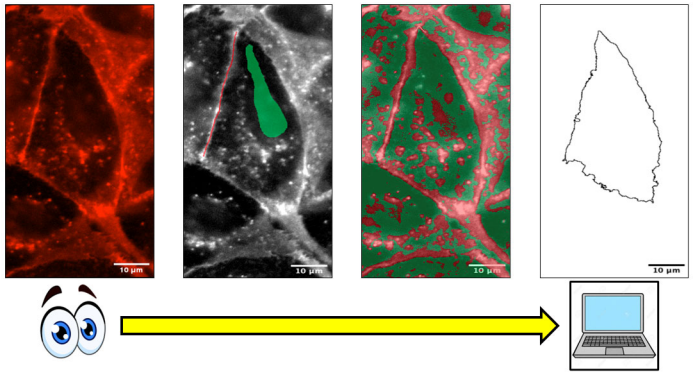

Cells are dynamic: they are constantly changing shape, stretching, contracting, dividing, and dying. Taken as a whole, these events define healthy versus unhealthy organisms, but there are not many high-throughput methods for scientists to measure and quantify these descriptive traits through time using live cells. The purpose of this study is to utilize image analysis software to quantify cell area, perimeter, velocity, and the tension force experienced by the cell. Once we have a robust and partially automated quantification method, we can test whether a possible mechanosensing protein, obscurin, affects cell mechanics.

Synthesis of N-Pyrazolylpropanoate Derivatives as Potential Ligands with Palladium

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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)PdCl2 formed Cl2Pd(L1 or L2)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 being stable in solution but with L1, a trans/cis isomerization is observed.

Evolution of Volatile Flavor Compounds Produced During the Fermentation of Beer with Genetically Different Yeasts

Andrew M. P. Roberts[1], Eliana M. Diaz-Aceituno[1], Juan M. Garcia[1], Angelina V. Lo Presti[1], Kayla Moore[1], Viridiana Tirado[2], Dr. Steven Harper[3], Dr. Samuel A. Morton[3], and Dr. Christine A. Hughey[1]
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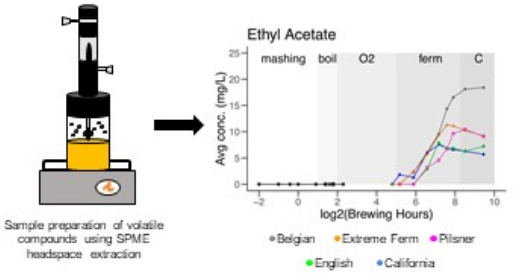

Beer is a complex mixture of volatile and nonvolatile compounds that arise from malt, hops, and fermentation. A pale ale wort brewed from a 2-row malt and Cascade hops was equally divided and fermented with genetically different yeast: WLP 001 California Ale, WLP 002 English Ale, WLP 566 Belgian Saison, WLP 800 Czech Pilsner Lager, and Wyeast 4347 Extreme Fermentation. While mashing and boiling samples were collected, this work focused on fermentation, the production of flavor compounds, and the differences across yeast strains. The Belgian and California yeasts began fermentation faster than other strains (e.g., within 12 hours of pitching) based on CO_2 bubbling. The Extreme Fermenter began production around 20 hours. The English ale and Pilsner started to produce flavor compounds ~40 hours and ~65 hours into fermentation, respectively. All fermentation tanks were within each yeast's optimal temperature range (20-23 ℃) except for the Pilsner, a lager yeast. All yeast produced the same compounds but in statistically different amounts, yielding different flavor profiles in the final beers. The Belgian produced the greatest amount of small yesters such as ethyl acetate and 2-methyl and 3-methyl butyl acetate. Pilsner produced the most medium-sized esters, which include ethyl heptanoate and ethyl octanoate. Extreme Ferm produced the most large-sized esters like ethyl nonanoate and ethyl dodecanoate. This research will help brewers understand how yeast strain selection impacts flavor and aroma development throughout the brewing process and in the final product.

An Affordable 3D-Printed UV Spectrophotometer

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Liquid chromatography systems are relatively expensive for undergraduate education and research. The price ranges are typically in tens of thousands of dollars. To more broadly introduce liquid chromatography methods and principles to education and research we are developing a modular open-source chromatography system. In this presentation, we describe our results on building and testing a UV detector at 280 nm for protein quantification. We used tinkercad, an online 3D modeling software with a simple and easy-to-learn interface to design structural pieces of a flow cell, and used 22 mm coverslips to provide UV-light access to the sample. We use an LED with a narrow emission spectrum centered at 280 nm to avoid costs and complications associated with using conventional mercury and deuterium lamps. The light intensity is measured with a UV photodiode and digitized with an Arduino board, and the single wavelength absorption allows us to avoid complex and expensive light-focusing lenses or mirrors. The data is transferred to a computer in real-time and analyzed with LabVIEW. To improve the signal-to-noise ratio and minimize data transfer bandwidth limits we oversample our output, average 500 data points, and transfer the averaged data. A set of performance benchmarks has been completed. We estimate that the cost of our detector is approximately $70 vs. >$2,000 for commercially available units. With this project, we hope to provide easy-to-follow instructions for others to build their own UV spectrophotometers and to incorporate them into undergraduate curriculum and research.

Structural Modeling and Analysis of β-amylase 9

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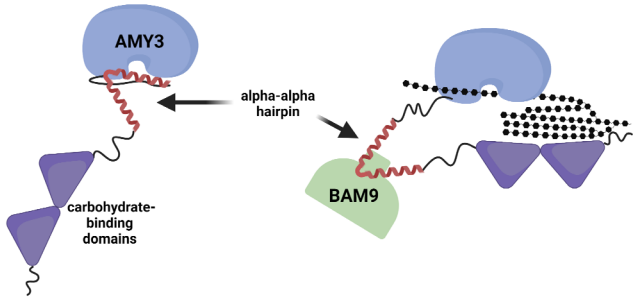

Starch, a polysaccharide glucose chain, is the food that plants make for themselves, and the plants it comes from help make up part of the global food source. The β -amylase family is a group of enzymes that catalyze starch degradation processes. β-amylase 9 (BAM9) is found in starch-containing plants, especially in Arabidopsis thaliana, and has been linked to the self-regulation of starch production in them. Even so, there is very little known about how BAM9 actually affects the starch degradation process. BAM9 is also currently thought to be in the class of pseudoenzyme, as it has thus far not been shown in literature to have any catalytic activity. α-amylase (AMY3) is a related enzyme that has been shown to be catalytically active in the starch degradation processes in plants. Recent two-hybrid assays and size exclusion chromatography experiments have suggested an interaction between BAM9 and AMY3. It is unclear why and where BAM9 and AMY3 interact and a better understanding of how this protein affects the vital process of starch regulation is incredibly important for the future of food stability and genetic engineering. There are currently no structures of BAM9 or known functions of it within the starch degradation process. To address this issue, a model structure of BAM9 was generated using AlphaFold2 in order to predict possible binding sites and interactions with other molecules involved in the starch degradation process. We then performed a series of OpenMM molecular modeling simulations using this proposed structure to describe the dynamics of the protein and how interacting partners affect these motions. As BAM9 showed potential catalytic activity with AMY3, interactions of BAM9 with AMY3 were modeled to show how these proteins interact and suggest a possible activation mechanism. Two potential interaction sites have been identified and are being tested experimentally. These data will provide the structural basis for a regulatory mechanism by BAM9 for AMY3 mediated starch degradation.

Morphological Studies of TiO_2 Nanoparticles on Au(111)

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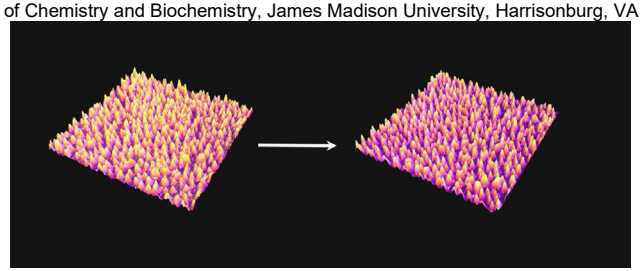

TiO_2 nanoparticles (NPs) supported on Au(111) form an inverse model catalyst that is active for alcohol oxidation and reduction. To fully understand the influence that the nanoparticle size and structure have on alcohol reactivity, TiO_2/Au(111) catalysts were synthesized and characterized. TiO_2 NPs were deposited on Au(111) in an O_2 background under ultrahigh vacuum (UHV) conditions. The reactivity of the TiO_2/Au(111) was tested using butanol temperature programmed reaction spectroscopy (TPRS). Two TiO_2 deposition times were studied, resulting in TiO_2 coverages of 0.13 ML and 0.27 ML, as determined by atomic force microscopy (AFM). In addition to quantifying TiO_2 coverages, the morphology and distribution of TiO_2 NPs were observed with AFM. To obtain the clearest images possible, the TiO_2/Au(111) samples were briefly annealed with a H_2 flame to clean contaminants from the surface. While a brief H_2 flame anneal does not affect the TiO_2 morphology, longer flame anneals cause changes in the morphology that are possibly consistent with the formation of a mixed metal oxide. With longer TiO_2 deposition time, the TiO_2 coverage increased, but particle size remained the same. Interestingly, the higher coverage of TiO_2 resulted in more consistent reactivity with butanol isomers, whereas the smaller coverage of TiO_2 NPs showed low reactivity. AFM results suggest that the difference in reactivity is likely due to the lower number of particles rather than to differences in the size and shape of TiO_2 NPs. These results help to inform the design of more active catalysts for alcohol partial oxidation.

Overcoming Degradation: A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs

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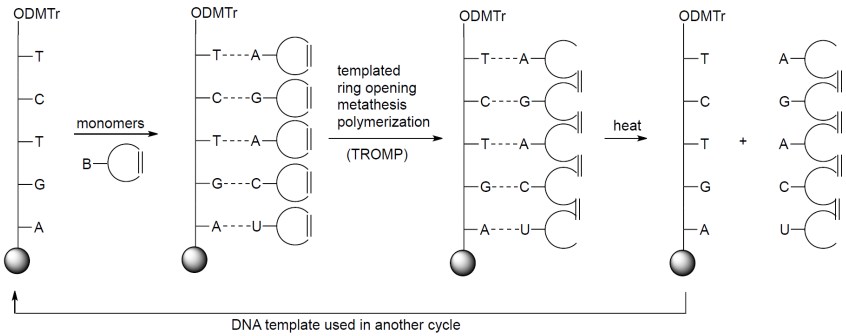

Antisense oligonucleotide analogs (ASOs) are short synthetically crafted or modified pieces of DNA or RNA that can attach themselves to existing messenger RNA (mRNA) to prohibit protein synthesis. Such molecules could be used to prevent unwanted protein production in existing cells or organisms. This would allow for the future prevention of protein and ribosome-based diseases in humans and possibly reduce the antibiotic resistance of bacterial organisms. The challenges faced by ASOs are a lack of stability, little defense against exonuclease compounds, and as a result a poor shelf life. To combat these complications novel synthetic pathways to form 7-membered rings were performed. Rings containing the bases Adenine, Cytosine, Thymine, Guanine, and Uracil have been successfully created. Additionally, a new focus on a possible 9-membered ring is underway.

"What RcoM Sees:" Investigating Potential Binding Domains for the DNA Complex of the Px-RcoM-1 Transcription Factor

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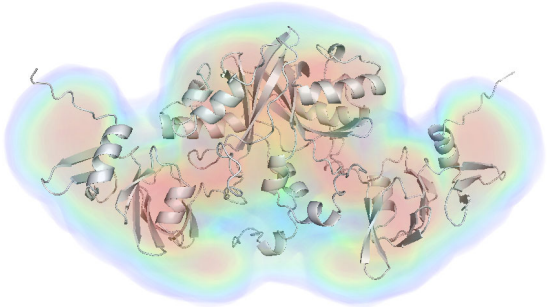

Bacteria must sense gases within their environment to efficient conduct metabolism and adapt to their environment. Bacteria utilize specific proteins that recognize the gases in the environment and these sensors regulate the transcription of metabolic genes. Paraburkholderia xenovorans, a bacteria that is studied for its ability to metabolism environmental pollutants, uses the protein RcoM to sense CO gas. RcoM has two functional domains, the DNA binding LytTR domain and a heme domain which binds to CO. While RcoM is a LytTR containing protein that uses DNA as a promoter, it is unique from many other LytTR containing proteins that bind dimeric promoters because RcoM does not recognize double or single repeat DNA sequences. Instead, RcoM binds a triplet repeat DNA sequence and requires two dimers. With this in mind, we sought to determine what the DNA binding mechanism is for RcoM. We collected SEC-SAXS data on RcoM, promoter DNA, truncations of RcoM, and RcoM mixed with the DNA. Calculated electron densities have informed the three-dimensional arrangement of the two domains. While it was difficult to produce a clear structure of the complex through ab initio model, we concluded that more than one RcoM binds to the DNA.

Quantifying cellular mechanics using time-lapse fluorescent microscopy

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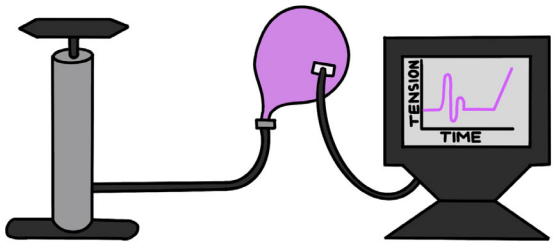

Cells constantly sense and react to their environment. To monitor their physical location and status within their environment, cells can use specialized cytoskeletal proteins to assess if the cell is under physical stress or strain and transmit that physical information in a biochemically significant signal. A giant cytoskeletal protein, obscurin, is one potential candidate for transmitting physical information into signals. Obscurin is expressed in low levels in most cells, yet cells that lose obscurin function tend to become cancerous. This is accompanied by increased motility and decreased cell adhesion. Obscurin acts as a connector in cells, linking distal regions to each other, and in turn, is functionally and structurally situated to act as a mechanosensor. Our lab is trying to probe this function more directly. While others in our lab are developing techniques to monitor how obscurin responds to physical forces, we are developing a pipeline to quantify cell dynamics, with the ultimate goal of monitoring how changes in obscurin affect cell architecture, motility, and membrane dynamics.

2023 Department of Chemistry and Biochemistry Student Award Winners

Amenta Award	Stuart A. Regitz
R.D. Cool Award	Ava J. Galgano
J.W. Chappell Scholarship (May 2022)	Taylor E. Bolt
Palocsay Award in Undergraduate Research	Zach D. Ryan
Service Awards	Will R. Hemmingson
J. W. Chappell Award	Quinn C. Harkrider
American Institute of Chemists	Jack W. Christman
Degesch America Award	Will R. Hemmingson
ACS Award	Amanda R. Cicali
Casali Scholarship (May 2022)	Connor J. Pearson
Dean's Award (Chemistry)	Connor J. Pearson
Dean's Award (Biophysical Chemistry)	Roujon A. Nowzari
CRC First Year Student Award	Sara E. Scanlan
NOBCChE Dr. Iona Black Award	Gabriella M. Newsome
Goldwater Scholars	Ava Galgano
	Stephanie Ouderkirk
Phi Beta Kappa	Catherine Besachio
	Will Hemmingson
Outstanding Student Researcher Award	*to be announced*

Divisional Awards

Biochemistry Award	Christine N. Buchholz
ACS Analytical Award	Drew M. Roberts
ACS Environmental Award	Shyleigh A. Good
ACS Inorganic Award	Stuart A. Regitz
ACS Organic Award	Connor J. Pearson
ACS Physical Award	Zachary D. Ryan

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