



College of Science and Mathematics

2024 REU SUMMER SYMPOSIUM

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY
DEPARTMENT OF GEOLOGY & ENVIRONMENTAL SCIENCE
DEPARTMENT OF PHYSICS & ASTRONOMY

THURSDAY JULY 25
&
FRIDAY JULY 26

Keynote Speaker



Rachel Stegmeier
(JMU Class of 2022)

Ph.D. Student, University of Virginia
Charlottesville, VA

After graduating from JMU with a degree in Chemistry and minors in Math, Spanish, and Honors Interdisciplinary Studies, I participated in the Fulbright Program as an English Teaching Assistant in Santiago de Compostela, Galicia, Spain at CIFP Compostela. This experience provided valuable insights and influenced my decision to pursue a PhD at UVA in Dr. Andreas Gahlmann's lab. In this keynote, I will share how I made the decision to pursue Fulbright before graduate school, the transformative experiences during my time in Spain, and the professional and personal growth that resulted. The session will highlight the benefits of alternative learning paths and international collaboration after completing an undergraduate degree, as illustrated by my Fulbright experience.

Thursday, July 25th

Multi-Slides Presentations I: EnGeo 2301		
9:00 am	Welcome Remarks	Dr. Steve Whitmeyer, Associate Dean for Research & Scholarship
9:10 am	<u>Lucas Brauchli</u> , and Dr. Thomas C. DeVore	Investigating Thermal Chemical Energy Storage with Iron(II) Sulfate
9:25 am	<u>Oliva Coer</u> , <u>Brandy L. Davidson</u> , Dr. Brycelyn Boardman, and Dr. Gretchen M. Peters	Tuning Plasticization of Chitosan Films with Boric Acid
9:40 am	<u>Mitchell Gelband</u> , Dr. Jason Czak	Quantification of Branching Behavior Under an Applied Electric Field in Reaction-Diffusion Systems
9:55 am	<u>Carter R. Johnson</u> , Ashley L. Corcoran, Enow S. Otto Jr., Dr. Nathan T. Wright, and Dr. Adebowale Ogunjirin	Determination of Affinity of Ligands for Polo-like Kinase 1 Polo-box Domain (PLK1 PBD) using Fluorescence Polarization
10:10 am	<u>Elanor Kirkland</u> and Dr. Isaiah Sumner	Computational Molecular Modeling between Glucosamine and Varying Plasticizers
10:25 am	Break	
10:40 am	<u>Sam Robinson</u> , <u>Griffin Keightley</u> and Dr. Chris Hollinsed	Synthesis of Contractile Polymers from Indicator Dyes
10:55 am	<u>Caitlin A. Gutierrez</u> and Dr. Brycelyn Boardman	Understanding the Aggregated Induced Emission of Quinazoline Derivatives in the Presence of Glucosamine and Chitosan
11:10 am	<u>Faith Stover</u> , <u>Sam Pearne</u> , <u>Zishaan Mahmood</u> , <u>Daniel Gass</u> , Dr. I Niculescu, Dr. G Niculescu	CLAS12 FTOF Efficiency Software: Developing User-Friendly Analysis Tools
11:25 am	<u>Hung Quach</u> , Valeri Krasheninnikov, Tai Quach, and Dr. Kevin L. Caran	Synthesis and Characterization of a Novel Polycationic, Hydrophobic, Antimicrobial, Water-Purifying Polymer
11:40 am	<u>Charles Beattie</u> , Alex Kline, Issac Spicher, Addison Shenk, Dr. Kristopher Schmidt, Dr. Timothy Bloss, Dr. Marquis Walker, and Dr. Giovanna Scarel	Radio waves Effect on the Nematode Caenorhabditis Elegans
11:55 – 1:00	Break	

Poster Session: King Lobby	
1:00 - 2:00 pm	Group A
2:00 - 3:00 pm	Group B

Poster Session: Group A	
<u>Juana Al Anbari</u> and Dr. Nathan T. Wright	Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation
<u>Yasmin Al Anbari</u> , <u>Stephanie N. Ouderirk</u> , and Dr. Nathan T. Wright	Measuring Cellular Mechanics via Image Analysis Techniques to Uncover a Molecular Pathway Involving Obscurin
<u>Sofia Barrows</u> , Iralis Cruz, Dr. Ángel García	LiDAR Mapping High Resolution Point Clouds in Butler Cave <u>Sofia Barrows</u> ¹ , Iralis Cruz ² , Dr. Ángel García ²
<u>Harrison P. Cancino</u>	Geomechanical Characterization of Mafic and Ultramafic Rock in Virginia for Carbon Mineralization Analysis
<u>Katy Carnes</u> , Dr. Ángel García, Dr. Dan Doctor	Analyzing Connections Between Grand Caverns and Fountain Cave
<u>Ashley L. Corcoran</u> , Carter R. Johnson, Enow S. Otto Jr., Dr. Nathan T. Wright, and Dr. Adebowale Ogunjirin	Evaluation of Binding Affinity of Novel Ligands at Polo-like Kinase 1 Polo-box Domain
<u>Mollie M. Corbett</u> , James T. Whitted, Dr. Ashleigh E. Baber	Modifying the Surface of Cu(111) to Drive Selective Oxidation Reactions
<u>Iralis Cruz</u> , Sophia Barrows, Dr. Ángel García, Dr. Ángel Acosta	Constructing High-Resolution Point Clouds of Butler Cave
<u>Emily Euler</u> , Haley Frankovich, Dr. Kendra Letchworth-Weaver and Dr. Ashleigh E. Baber	Computationally Enhanced Investigation of Reactivity of Isomeric Butanol on TiO ₂ /Au(111)
<u>Elijah Fernands</u> , Frank Muscarella, Dr. Lindsay Caesar, Diana Northup, Paris Salazar-Hamm	Induction of Secondary Metabolites in Bat-associated Bacteria using SAHA to Fight White-Nose Syndrome
<u>Summer Kantanen</u> and Dr. Jason Czak	The Effects of Perturbations in Feed Parameters with Spatially Localized Functional Forms on Reaction-diffusion Systems
<u>Bianca P. Maldonado</u> , Dr. Ángel A. García, and Dr. Angel A. Acosta	Characterizing Rare Speleothems: Resuming the Conversation about Shields Formation
<u>Christian Orrico</u> and Dr. Anca Constantin	Towards A Better Understanding Of The Relationship Between Black Hole Accretion And Maser Emission Via Mid-Infrared Variability Structure Function
<u>Enow Otto Jr.</u> , Carter Johnson, Ashley Corcoran, and Dr. Adebowale Ogunjirin	Accelerated Binding Affinity Determination using Fluorescence Polarization
<u>Ruhi Rahman</u> and Dr. Christopher Berndsen	Characteristics of Carbohydrate-binding Module of the alpha Amylase AMY3
<u>Ian Spurgeon</u> and Dr. Isaiah Sumner	Quantum Oscillator and Particle-in-a-box models with Google Colab
<u>Jackson Tester</u> and Dr. Chris Berndsen	Pseudoenzyme LIKE SEX FOUR 1 Has Little Effect on Beta Amylase Hydrolysis Activity
<u>James T. Whitted</u> , Mollie M. Corbett, Dr. Ashleigh E. Baber	Exploring the Epoxidation of Isoprene on Copper-Based Catalysts
<u>Ethan Zimmerman</u> , <u>Owen Paulson</u> and Dr. Klebert Feltosa	Impact of Particle Morphology, Preparation Method and Confinement on the Angle of Repose for Granular Materials

Poster Session: Group B	
<u>Daphne M. Antwi, Kalany N. Santos-González</u> , Dr. Gina MacDonald	Amino Acid Influences on Lysozyme Structure, Stability, and Aggregation
<u>Trip Beaver</u> , Dr. Chris Berndsen	Malate Dehydrogenase and Like Sex Four 1 Activities Affected by Varying Concentrations of Starch
<u>Trevor Brown, Kamryn McGary</u> , David Lawrence, Costel Constantin and Masoud Kaveh	Optical and Microscope Characterization of Gd-doped ITO Thin Films
<u>William Brown</u> , Eric Shepard, Tengis Tamir and Dr. Debra Mohler	Creation of a Synthetic Strategy for Novel Antisense Oligonucleotide Analogs
<u>Olivia E. Coer</u> and Dr. Brycelyn M. Boardman	Modulating the Properties of Chitosan Films with Polyol-Boric Acid Complexes
<u>Brandy L. Davidson</u> and Dr. Gretchen M. Peters	Structural Determination of Polyol-boric Acid Complexes using NMR Spectroscopy
<u>James Fuller</u> , Ricky Gonzales, Pedro Rivera, Dr. Shane McGary	How Effective Electrical Resistivity is as Maze Caves Form at Deeper Depths in Butler Cave
<u>Emma J Goehner, Stephanie J Schwender, Lewis D. Crooks IV</u> , and Dr. Barbara Reisner	Exploring Nanocellulose as a Matrix for Metal Organic Framework Composites
<u>Ricky Gonzales</u> and R Shane McGary	Finding Approximate Locations for Cave Systems using Electrical Currents
<u>Anna Grove</u> and Gretchen Peters	Impacts of Gronic Acid on the Properties and Function of Supramolecular Peptide Gels
<u>Frances E. Homan</u> , Shyleigh A. Good, Mary M. Sessoms, and Dr. Lindsay K. Caesar	Induction of Natural Products by Fungal-Fungal Co-cultures
<u>Catherine Hughes</u> , Dr. Dhanuska Wijesinghe	Variability of Physical and Geochemical Properties of Cave Ecosystems: A Case Study in Water Sinks Cave, Highland County, VA
<u>Luke McFather</u> , Dr. Jon Monroe, Dr. Christopher Berndsen	Characterizing the Interaction between the Amylases BAM9 and AMY3
<u>Kamryn McGary, Trevor Brown</u> , David Lawrence, Costel Constantin and Masoud Kaveh	Fabrication of Gd Doped ITO Thin Films
<u>Kayla H. Moore</u> and Dr. Brycelyn M. Boardman	The Importance of Polyol Structure: A Spectroscopic Investigation of Triols and Linear Polyols Interaction with Glucosamine and Chitosan
<u>Estrella Rayner, Carson Wilkinson</u> and Gina MacDonald	Circular Dichroism and Infrared studies of Amino acid influences on Bovine Serum Albumin Structure and Aggregation
<u>Pedro Rivera</u> , Bryan Crowell, Dr. Dhanuska Wijesinghe and Dr. Shane Mc. Gary	Analysis of Cave Sediments and Morphological Controls on Deposition, Butler Cave, Burnsville Cove, Virginia
<u>Cadence Russell</u> , Dr. Yonathan Admassu, and Dr. Dhanuska Wijesinghe	Automated Sinkhole Mapping with ArcGIS Using Shape Factors in Harrisonburg, VA
<u>Sara E. Scanlan</u> , Dr. Jonathan D. Monroe and Dr. Christopher E. Berndsen	Development of a Colorimetric Assay to Test Amylase Activity

Thursday, July 25th

Multi-Slides Presentations II: EnGeo 2301		
3:10 pm	<u>Grace Chamberlain</u> , Lily Jade Joyce, and Dr. Kendra Letchworth-Weaver	Computational Investigation of High Entropy Oxides
3:25 pm	<u>Stephan Simons</u> and Dr. Chris Hughes	Indium Modification of Self-Assembled Monolayers
3:40 pm	<u>Kyle Shipman</u> and Dr. Adebawale Ogunjirin	Synthesizing Nicotinic Analogue to Inhibit PLK 1 PBD
3:55 pm	<u>Angelina M. Sardelli</u> , Dr. Christopher E. Berndsen	Environmental Effects on the Mechanism of Starch Cleavage in beta-amylases
4:10 pm	<u>Katelyn Bowers, Dylan Virts</u> , and Dr. Christine Hughey	Identification, Validation, and Quantitation of Unknown Metabolites in SMAsh beer using Molecular Networking

Friday, July 26th

Keynote Speaker: EnGeo 2301		
9:00 am	Rachel Stegmeier ('22)	<i>Exploring Alternative Paths: My Fulbright Experience in Spain and Its Impact</i>
10:00 am	Break	

Multi-Slides Presentations III: EnGeo 2301		
10:15 am	<u>Elaina X. Manyin</u> and Dr. Isaiah Sumner	Glycerol Boric Acids Interacting with Glucosamine
10:30 am	James Love, Jr, Mikayla Picardo, <u>Aidan Pisarcik</u> , Dr. Gabriel Niculescu, and Dr. Ioana Niculescu	Building and testing a Cosmic Ray Telescope for Micro-Pattern Gas Detector Characterization
10:45 am	<u>Eric J Shepard, Tengis Tamir</u> , and Dr. Debra Mohler	A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs
11:00 am	Break	
11:15 am	<u>Patrick T. Randolph</u> and Dr. Thomas C. DeVore	Acetone's Abnormal Relaxation Time Trend is a Result of Dissolved Oxygen
11:30 am	<u>Emma J Goehner, Stephanie J Schwender, Lewis D. Crooks IV</u> , and Dr. Barbara Reisner	Dye-ing to Learn: Understanding the Chemistry behind CHEM 132L Water
11:45 am	<u>Jakeline Veliz Diaz</u> and Dr. Keigo Fukumura	Coupling between X-Ray Obscuration and UV Absorption by AGN Accretion Disk Winds
12:00 am	Recognitions and announcements	

STUDENT ABSTRACTS

Multi-Slide Presentations: Session I

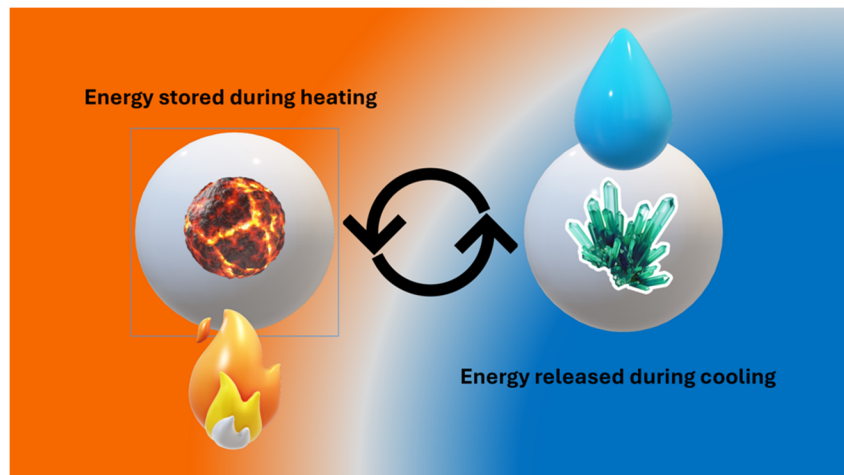
(Student presenters underlined)

Investigating Thermal Chemical Energy Storage with Iron(II) Sulfate

Lucas Brauchli, and Dr. Thomas C. DeVore

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

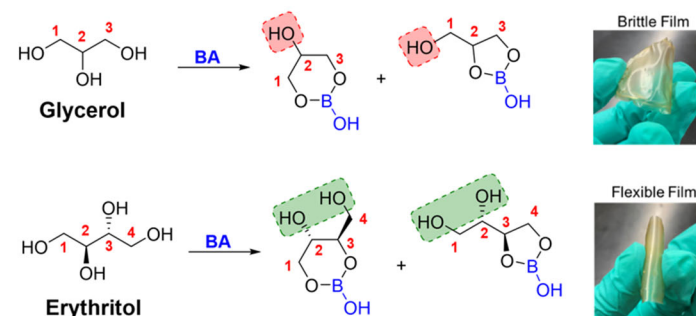
This study investigates the thermodynamic properties of iron(II) sulfate, a salt hydrate that can exist in the heptahydrate form ($\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$) and the tetrahydrate, monohydrate, and base form. The significance of this process with this compound is that it can be cycled for renewable energy while also being paired with applications in water recovery. This investigation includes an analysis of its crystal structure, hygroscopic tendencies, and thermal behavior. Characterization techniques including powder X-ray diffraction (PXRD) and Infrared Spectroscopy (IR) were used to determine composition and structural changes. Differential scanning calorimetry (DSC) was used to analyze enthalpy changes during the dehydration process while thermogravimetric analysis (TGA) was used to calculate the mass loss over the dehydration process. Samples of $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ were dehydrated in an oven (~110C) and in a furnace (300C) and rehydrated in a humidity chamber. Mass measurements were taken periodically to determine the amount of water each sample gained/lost. In addition, once dehydrated, Iron(II) gets converted to iron(III) which creates the compound $\text{Fe}(\text{OH})(\text{SO}_4)$ which could be a potential candidate for water collection since it displays hygroscopic behavior relatively quickly. Promising applications in clean energy can be explored where endothermic heat released and exothermic heat gained can be cycled for renewable energy in cold seasons.



Tuning Plasticization of Chitosan Films with Boric Acid

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

Chitosan-based bioplastics are attractive biodegradable alternatives to petroleum-derived plastics. However, optimizing the properties of chitosan materials with plasticizers to fit particular applications remains a significant challenge. Here, we report the ability to control the binding potential of alcohol-rich plasticizers with boric acid. In the presence of boric acid, polyol plasticizers form neutral complexes that alter the hydrogen-bonding face of the plasticizer, resulting in changes to the effectiveness of the plasticizer. In our previous work with glycerol, we found that the formation of glycerol-boric acid complexes yielded chitosan films that were less flexible, had increased thermal transition temperatures, and showed more uniform morphologies. Longer polyols, such as erythritol and its stereoisomers, D- and L-threitol, also form neutral complexes with boric acid. In these complexes, however, a free diol unit is present. As a result, films containing erythritol- or threitol-boric acid complexes showed an increase in both thermal stability and flexibility. Structural, thermal, mechanical and morphological characterization was performed using ATR-FTIR, TGA, DMA, and SEM. Molecular-level interactions of the neutral boron complexes and D-glucosamine (GlcN), the repeat unit of chitosan, were also investigated using NMR and ATR-FTIR. These results highlight the interactions between the NH and OH functionalities of GlcN and the free OHs of polyol-boric acid complexes. The combined results demonstrate the necessity of specific hydrogen-bonding interactions between the plasticizer and the polymer for effective plasticization, an important insight into the plasticization mechanism of chitosan films.



Quantification of Branching Behavior Under an Applied Electric Field in Reaction-Diffusion Systems

Mitchell Gelband, Dr. Jason Czak

Department of Physics, James Madison University, Harrisonburg, VA 22807

Reaction-diffusion systems are renowned for their capability to generate spatio-temporal patterns. The Gray-Scott model, in particular, has been observed to exhibit a variety of patterns including stationary pulses, traveling pulses, self-replicating pulses that form branching and coarsening behavior, up to chaotic behavior. Utilizing a peak detection method that identifies peaks by simple neighboring relationships in addition to the ability to detect saddle points in data enables the quantification of self-replicating behavior within these systems. Furthermore, peak detection facilitates initiation in the analysis on the influence of an applied electric field in a Gray-Scott-like system by finding the drift velocity of the pulses in simpler regimes.

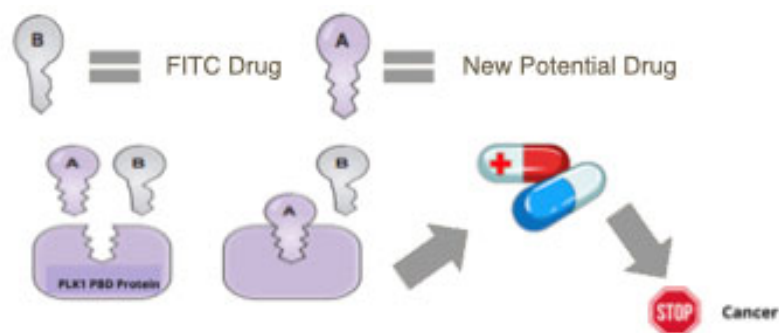
Determination of Affinity of Ligands for Polo-like Kinase 1 Polo-box Domain (PLK1 PBD) using Fluorescence Polarization

Carter R. Johnson², Ashley L. Corcoran², Enow S. Otto Jr.², Dr. Nathan T. Wright¹, and Dr. Adebowale Ogunjirin²

¹Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

²School of Science, Technology, Accessibility, Mathematics and Public Health, Gallaudet University, Washington DC 20002

Cancer is a disease with a generally low survival rate, and can affect 1 in 3 individuals. Current drugs often lack specificity, highlighting the need for continued research into more targeted treatments. A critical step in the drug discovery process is determining the affinity of potential drug molecules for their targets, such as the polo-like kinase 1 polo-box domain (PLK1 PBD), which promotes cancer cell proliferation. In this study, we used a Fluorescence Polarization approach to assess the affinity of over 40 drug molecules for PLK1 PBD. The results were analyzed by seeing how much the drug molecules inhibit FITC-Poloboxide from binding to the PLK1 PBD. Our results identified approximately 7 drug-like molecules with the potential to be developed into effective anticancer agents.

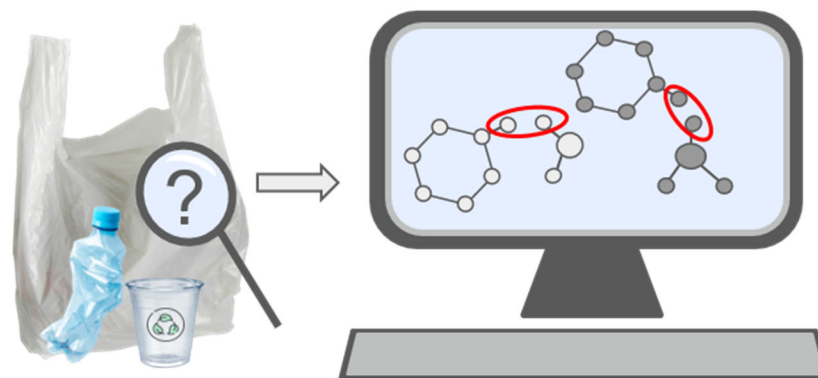


Computational Molecular Modeling between Glucosamine and Varying Plasticizers

Elanor Kirkland and Dr. Isaiah Sumner

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

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

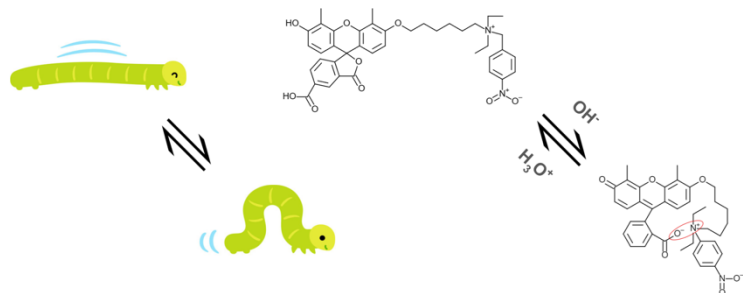


Synthesis of Contractile Polymers From Indicator Dyes

[Sam Robinson](#), [Griffin Keightley](#) and Dr. Chris Hollinsed

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

Novel materials with unique properties are always in demand, as applications abound for their usage. The Hollinsed lab group has attempted to create organic polymers capable of contracting and expanding for a variety of potential utilizations. The function of these molecules is to reversibly bend carbon chains in each monomer unit to decrease the total length of the polymer when exposed to basic conditions or electrochemical stimulus. This change is achieved through formation of a negatively charged oxygen in the 'ring open' form of the molecules, which attracts to the positively charged quaternary ammonium section of the monomer. These polymers were created through highly convergent synthesis from accessible reagents.



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

[Caitlin A. Gutierrez](#) and Dr. Brycelyn Boardman

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

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



CLAS12 FTOF Efficiency Software: Developing User-Friendly Analysis Tools

[Faith Stover](#), [Sam Peame](#), [Zishaan Mahmood](#), [Daniel Gass](#), Dr. I Niculescu, Dr. G Niculescu

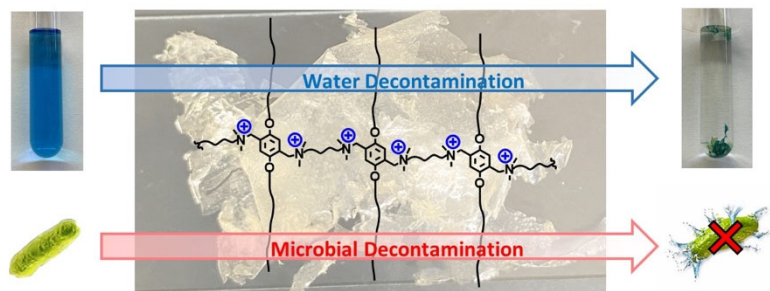
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

The CLAS12 Spectrometer in Hall B at the Thomas Jefferson National Accelerator Facility is a ~50 M\$ spectrometer built by an international consortium, including JMU. A critical component of this system is the Forward Time-of-Flight (FTOF) detector, an array of ~1200 plastic scintillators, which provides timing information for the whole detector. The core of this project is the development of software designed to analyze and document the efficiency of the FTOF components. Starting with the initial code developed by our Glasgow collaborators, the JMU group reworked the code using the MVC (Model View Controller) design philosophy. Results of these efforts will be showcased in this presentation.

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

Hung Quach, Valeri Krashennikov, Tai Quach, and Dr. Kevin L. Caran
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

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



Radio waves effect on the nematode *Caenorhabditis elegans*

Charles Beattie, Alex Kline, Issac Spicher, Addison Shenk, Dr. Kristopher Schmidt, Dr. Timothy Bloss, Dr. Marquis Walker, and Dr. Giovanna Scarel
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807
Department of Biology, Eastern Mennonite University, Harrisonburg, VA 22802
Department of Biology, James Madison University, Harrisonburg, VA 22807

Utilizing the LITE-1 and GUR-3 photoreceptors the nematode *Caenorhabditis elegans* (*C. elegans*) is able to respond to blue and ultraviolet light. Subsequent bombardment of radio waves as well as red and white light was used in order to further determine the effect of high energy long wavelength radiation on biological receptors. This was achieved by filming *C. elegans* as it underwent irradiation and then processing the video using Tierpsy tracking software. Usage of this method revealed that electromagnetic waves traditionally considered "low" energy can have a near equal effect on biological receptors.

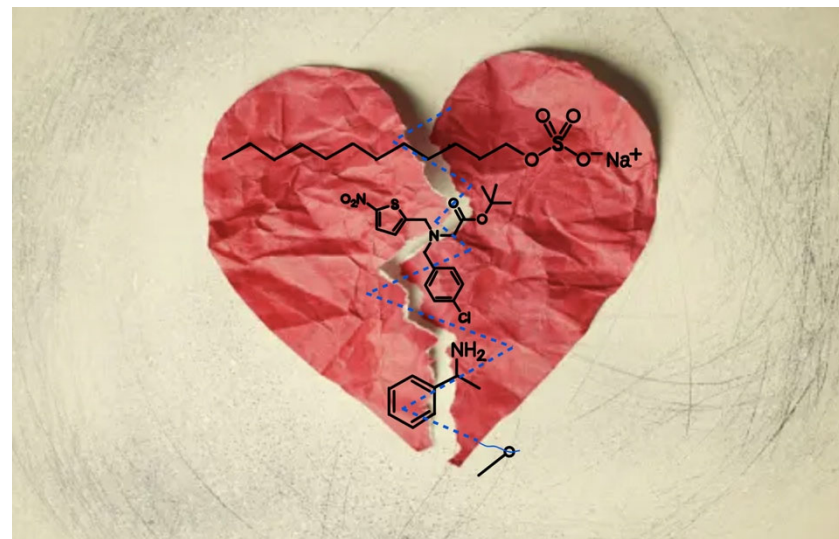
STUDENT ABSTRACTS Poster Session: Group A

Listed in alphabetical order by presenter's last name
(Student presenters underlined)

Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation

Juana Al Anbari and Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Desmoplakin is a protein in the desmosome that plays an integral role in connecting the intermediate filaments from one cardiomyocyte to another. Some desmoplakin mutations have been linked to arrhythmic cardiomyopathy and fragile skin disease. Specific mutations in DSP (R451G, S507F, S442F, and S299R) result in hypersensitive cleavage in the presence of the protease calpain. To block this cleavage event, we have screened drugs for their ability to specifically inhibit calpain-dependent DSP degradation. Here we begin studies designed to further interrogate the most promising 19 drugs for their ability to bind to DSP and for their ability to disrupt the calpain-DSP interaction. STD-NMR experiments show that 12 of the drugs bind to DSP in the μM range. SPR experiments show that calpain and DSP bind in the μM range, but this binding event has not yet been fully explored. Future work will focus on increasing the protein purification yield, optimizing the SPR experiment, and quantitatively assessing the various drug-DSP interactions.



Measuring Cellular Mechanics via Image Analysis Techniques to Uncover a Molecular Pathway Involving Obscurin

Yasmin Al Anbari¹, Stephanie N. Ouderirk², and Dr. Nathan T. Wright¹

¹Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

²Merck & Co. Inc., Elkton, VA 22827

Obscurin is a large cytoskeletal protein present in epithelial and muscle cells. When obscurin is knocked down or knocked out, epithelial cells undergo an epithelial-to-mesenchymal transition (EMT), a process linked to cancer development, accompanied by faster cell migration. Conversely, when select obscurin domains are added to epithelial cells, this results in decreased migration. From these and other data, it is now understood that obscurin inhibits migration through two separate pathways; the activation of the RhoA/ROCK pathway and the inactivation of the PI3K pathway. Here we study the interplay of these obscurin linked pathways. In a previously unstudied cells type (MDCK) the addition of the obscurin C terminus leads to decreased migration. Constructs where either the PH domain (responsible for PI3K signaling) or the RhoGEF domain (responsible for RhoA signaling) are removed also results in decreased migration, suggesting a redundant function. Surprisingly, the inhibition of both pathways still results decreased cell velocity which suggests the presence of a third motif of the obscurin C terminus that modulates motility. This is perhaps linked to obscurins colocalization with cytoskeletal/membrane connecting structures. To probe this potential new function in more detail we disrupted the cytoskeleton and found that obscurin crosslinks with intermediate filaments but not actin fibers. Taking together these results suggests that obscurin modulates cell velocity through at least three separate molecular mechanisms. Future work will focus on characterizing and delineating these pathways more clearly.



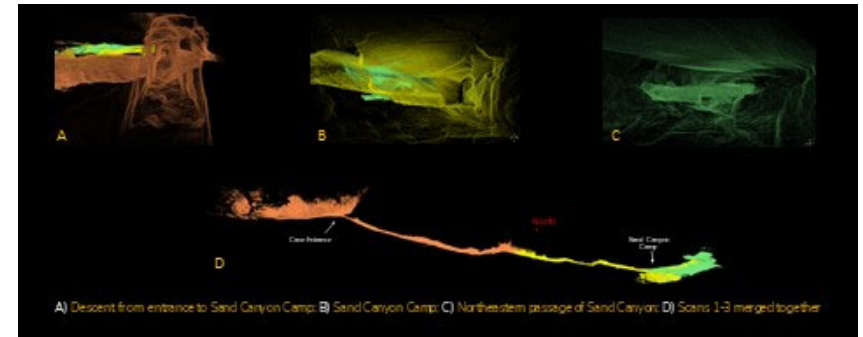
LiDAR Mapping High Resolution Point Clouds in Butler Cave

Sofia Barrows¹, Irnalis Cruz², Dr. Ángel García²

¹Department of Geology and Environmental Science, James Madison University, Harrisonburg, VA 22807

²Scripps Institution of Oceanography, University of California, San Diego

Traditional cave mapping provides essential spatial observations of cave morphology. The use of LiDAR in cave mapping expands applications beyond basic mapping to include fields such as stratigraphy, paleoclimatology, geomorphology, and hydrology. Butler Cave, located in west-central Virginia near the Appalachian Mountains, encompasses many miles of explored passages within the Valley and Ridge Province, with numerous hydrological pathways created by the nearby James River. The outcrops at Butler Cave offer an excellent opportunity to observe the intersection of structural analysis, traditional mapping, and high-definition point cloud generation inside of caves. This project constructed multiple georeferenced high-definition point clouds of Butler Cave to create a 3D map. We produced an updated map for cavers, speleologists, and the Butler Cave Conservation Society (BCCS). The use of LiDAR-SLAM technology in cave mapping serves as a model for other research institutions and conservation efforts, demonstrating a non-destructive, efficient method for detailed cave exploration.



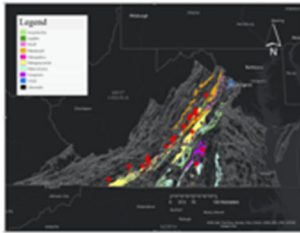
Geomechanical Characterization of Mafic and Ultramafic Rock in Virginia for Carbon Mineralization Analysis

Harrison Cancino¹, Maria Petrova¹, Jenny Meng², Yonathan Admassu¹

¹Department of Geology and Environmental Science, James Madison University, Harrisonburg, Virginia, 22807

²Virginia Department of Energy, Charlottesville, Virginia, 22903

Carbon mineralization, also known as carbon capture or carbon storage, is the process of injecting carbon dioxide from the atmosphere into rock masses below the surface of the Earth. In essence, this accelerates the carbon cycle and helps reduce carbon dioxide in the atmosphere. The formation of Magnesite ($MgCO_3$) is essential in the process of carbon mineralization where it naturally forms during the weathering of ultramafic rocks. By qualitatively characterizing masses of mafic and ultramafic rock on the scale of 10-100 meter outcrops, these masses can be rated for their suitability for carbon mineralization. To assist in this analysis, we created ~5cm cubic samples and tested their hardness using a Schmidt hammer and point load system. This data was collected and compared to help determine the suitability of different VA geologic formations for carbon mineralization. Results are pending.



Analyzing Connections Between Grand Caverns and Fountain Cave

Katy Carnes¹, Dr. Ángel García², Dr. Dan Doctor³

¹Department of Environmental Science and Geology, Berry College

²Department of Geology and Environmental Sciences

³Research Geologist, USGS

Fountain Cave and Grand Caverns sit beside each other at Cave Hill along the Shenandoah Valley in Virginia. Knowing the hydrological systems that these caves are connected to is important for better understanding their paleoclimates, and whether they have the same water source or not. Paleoclimate helps reveal the change in climate over time and can help predict how it will continue to change. Paying attention to precipitation is important to determine how much of a role, if any, it plays in drip rate by proving drip rate is higher during wet periods and lower in dry periods. If seasonality is not related to drip, then more hypotheses for what hydrological systems are connected to these caves can be tested. Oxygen isotopes can help interpret environmental controls, soil, epikarst, and the cave system as a whole.



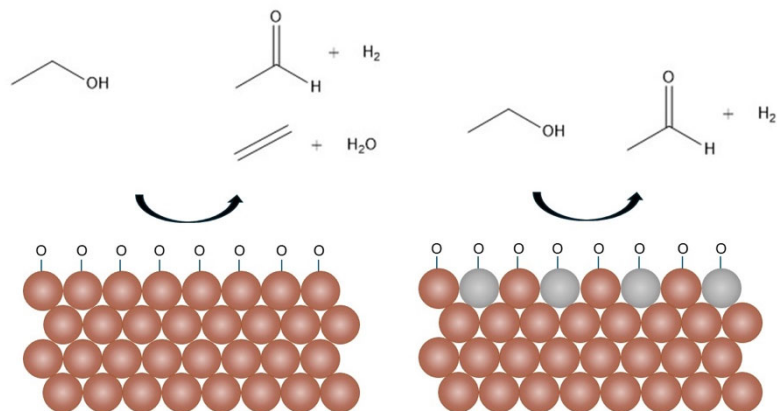
Figure 1. As the stalactite drips water, a rain gauge on a tripod collects the water to record drip events, temperature, conductivity, and relative humidity.

Figure 1.

Modifying the Surface of Cu(111) to Drive Selective Oxidation Reactions

Mollie M. Corbett, James T. Whitted, Dr. Ashleigh E. Baber

Aldehydes and epoxides are widely used in industrial, agricultural, transportation, construction, and medical settings. These compounds can be produced by exposing small alcohols and olefins to an oxidized metal surface. Previous work has investigated Cu(111) which is an excellent oxidizing agent, but it is not a selective catalyst for the desired products. Ag(111) has also been used, and despite being a selective catalyst for aldehydes and epoxides, it is not easily oxidized with atomic oxygen. Under ultrahigh vacuum (UHV) conditions, a bimetallic system can be utilized by exposing a Cu(111) surface to silver atoms, creating a surface that has optimized the desirable properties of both metals. This also reduces the need for promoters which are expensive and in some cases, toxic. Here, ethanol, ethylene, and propylene were used to study the production of aldehydes and epoxides. Temperature programmed desorption (TPD) experiments were used to study the reactivities of these molecules under different oxygen coverages. Oxygen was dosed at room temperature to form atomic oxygen on the surface of Cu(111) (O/Cu(111)). Ethanol on O/Cu(111) formed $82.24 \pm 3.49\%$ of acetaldehyde compared to ethylene and recombinative ethanol across all oxygen coverages (50-600 L). On the other hand, the olefins reacted 100% selectively to form combustion products (CO₂ and H₂O), which are the undesired products. Auger electron spectroscopy (AES) was used to monitor the deposition of Ag on Cu(111) which will be implemented to increase the selectivity of desired products – acetaldehyde from ethanol and epoxides of ethylene and propylene. Future TPD studies will be conducted to explore the reactivity of Ag/Cu(111) for selective oxidation reactions of alcohols and olefins.



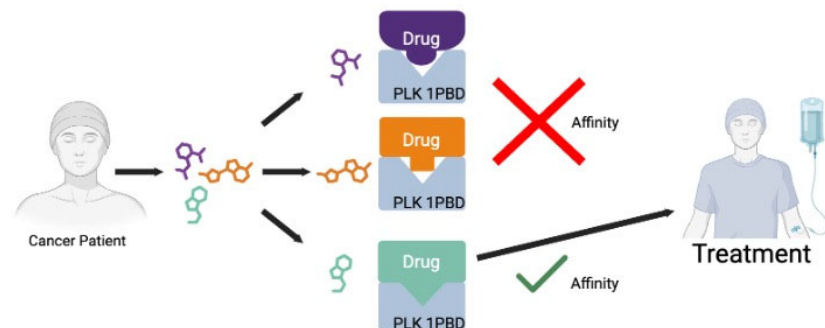
Evaluation of Binding Affinity of Novel Ligands at Polo-like Kinase 1 Polo-box Domain

Ashley L. Corcoran, Carter R. Johnson¹, Enow S. Otto Jr.², Dr. Nathan T. Wright¹, and Dr. Adebowale Ogunjirin²

¹Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

²School of Science, Technology, Accessibility, Mathematics and Public Health, Gallaudet University, Washington DC 20002

The search for effective cancer treatments often begins with identifying ligands that can target specific proteins involved in the disease progression. Here, we screened various synthesized ligands for their potential to bind to the Polo-like kinase 1 polobox domain (PLK1PBD) protein, known for its critical role in promoting cancer proliferation. We established and validated an in-house protocol to evaluate the affinity of 46 novel compounds towards PLK1 PBD. This screening process identified six compounds as promising candidates for further evaluation as potential leads in discovering novel anti-cancer drugs.



Constructing High-Resolution Point Clouds of Butler Cave

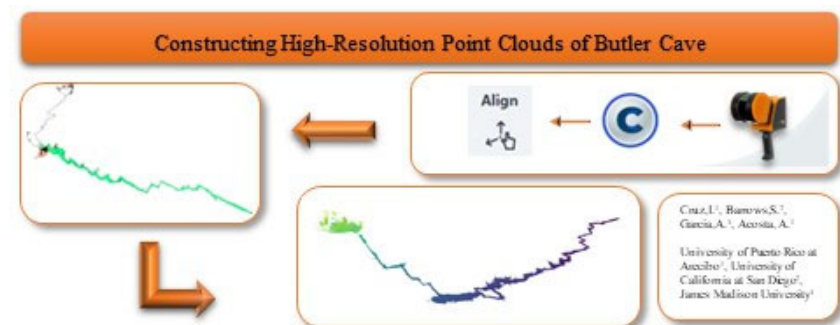
Irnalis Cruz¹, Sophia Barrows², Dr. Ángel García³, Dr. Ángel Acosta¹

¹Physics and Chemistry Department, Universidad de Puerto Rico at Arecibo, Arecibo, Puerto Rico

²Department of Geosciences, Scripps Institution of Oceanography, University of California at San Diego, California, USA

³Department of Geology and Environmental Science, James Madison University, Harrisonburg, Virginia, USA

The field of cave cartography has significantly advanced with the adoption of 3D topography using LiDAR technology. Butler Cave in Virginia was discovered in 1958, the geomorphology of the cave consists in an extensive natural underground passages and chambers. The most recent cave survey was in 1985 and produced a plan view map. Despite the years of study of this cave, a comprehensive 3D map of the cave system has not been created. Therefore, our study aims to produce a 3D map of Butler Cave using the handheld LiDAR Geoslam Zeb Horizon and produce a detailed high resolution cave map to assess cave deformation and its geomorphology. LiDAR technology uses infrared lasers that reflect off surfaces and return to the sensor, measuring the time of flight we can generate a geometrical representation of the cave and construct a high-definition point cloud. A millimeter resolution is obtained using the LiDAR and its capabilities (range is 100 meters, 300,000 scanner points per second and a rotating field of view). Post-data analysis includes using SLAM (simultaneous localization and mapping) technology to obtain the point cloud and since is a large cave, merging the different scans was required to complete the map. After the completion of the map, then the cave deformation analysis can be performed. Butler cave deformation is influenced by geological processes during formation, involves translation, rotation, and internal deformation, all of which can be analyzed using the 3D model. The final 3D product will be given to Butler Cave Conservation Society for future studies.



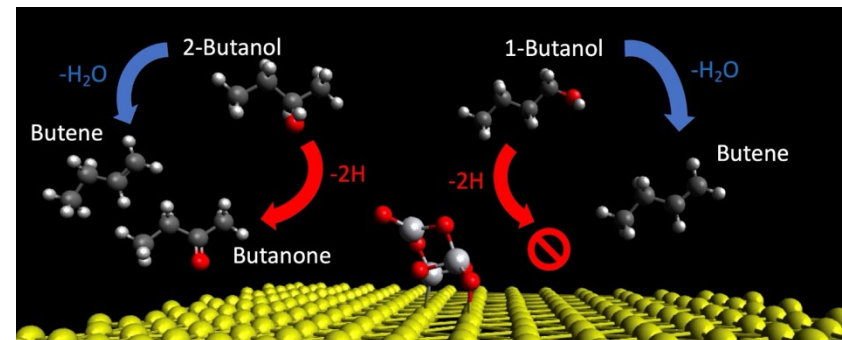
Computationally Enhanced Investigation of Reactivity of Isomeric Butanol on TiO₂/Au(111)

Emily Euler¹, Haley Frankovich¹, Dr. Kendra Letchworth-Weaver² and Dr. Ashleigh E. Baber¹

¹Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

²Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

Biofuels such as butanol can be utilized to minimize global fossil fuel reliance while contributing to a carbon-neutral cycle. Developing a deeper understanding of the fundamental thermal catalysis processes of butanol over heterogeneous model catalysts can aid in the design of more efficient catalysts. Temperature-programmed desorption (TPD) experiments demonstrate differences in both reactivity and selectivity for butanol isomers with 1-butanol showing little reactivity and only elimination products while 2-butanol shows both oxidation and elimination. To gain an atomically-detailed perspective on these processes, density functional theory (DFT) was used to investigate energetic trends and identify comparisons between 1- and 2-butanol as they adsorb on TiO₂ nanoparticles supported on a Au(111) surface. There are two favorable interactions between the butanol and the catalyst material; the oxygen on butanol covalently bonds to the nanoparticle and the alkane chain interacts with the gold surface through dispersion forces. Initial conclusions determine the adsorption energies of both 1- and 2-butanol to be less dependent on coordination number of the Ti and more dependent on gold surface interactions. Preliminary results indicate that there are more active sites available for 2-butanol to interact favorably with both the nanoparticle and the gold surface compared to 1-butanol, potentially influencing reactivity and selectivity. DFT calculations to further investigate the reaction pathways for 1- and 2-butanol elimination and oxidation are ongoing.

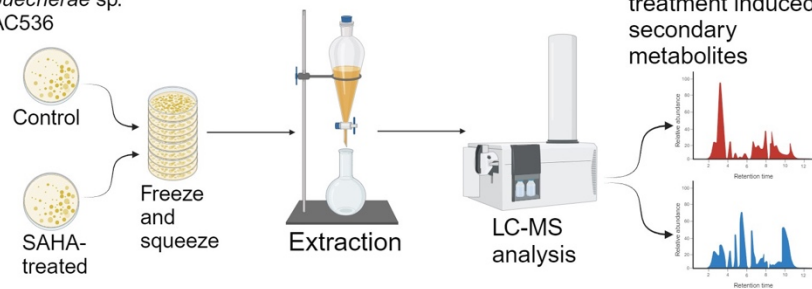


Induction of Secondary Metabolites in Bat-associated Bacteria using SAHA to Fight White-Nose Syndrome

Elijah Fernands¹, Frank Muscarella¹, Dr. Lindsay Caesar¹, Diana Northup², Paris Salazar-Hamm²,
¹Dept. of Chemistry and Biochemistry, James Madison University
²Dept. of Biology, University of New Mexico

Bat populations in the US continue to decline due to the fungus *Pseudogymnoascus destructans*, the species that causes White-Nose Syndrome (WNS). Over 7 million bats have died in the last decade from this disease, greatly harming ecosystems and agriculture. Fortunately, some caves are still WNS free, leading scientists to explore how bats living in these caves obtain protection from this disease. In a recent study, over 1,000 bacteria from WNS-free bats were isolated, and around 100 strains had antifungal activity against *P. destructans*. The compounds responsible for this activity were not identified. A pilot study from the Caesar lab on 18 bioactive strains from this study identified a set of target metabolites with putative antifungal activity. The most bioactive bacterium, *Streptomyces buecheerae* sp. AC536, was chosen for scale up growth for targeted isolation studies. Unfortunately, upon scale up growth, the target metabolites stopped being produced, most likely due to a lack of required environmental triggers in a laboratory setting. Bacterial biosynthetic pathways are under strict transcriptional regulation so that energetically expensive products are only formed when they are likely to provide a competitive advantage. To reactivate these silent biosynthetic pathways, we tested different growth conditions that varied in temperature, light exposure, carbon source, and/or chemical additives. Interestingly, growth of AC536 in the presence of the histone deacetylase inhibitor suberoylanilide hydroxamic acid (SAHA) led to significant upregulation of secondary metabolites. There were major challenges in replicating unique or upregulated metabolites in the SAHA treatment. After several runs, there were six compounds consistently unique or upregulated in SAHA compared to control, and of those six all have been putatively identified using Natural Product Atlas.

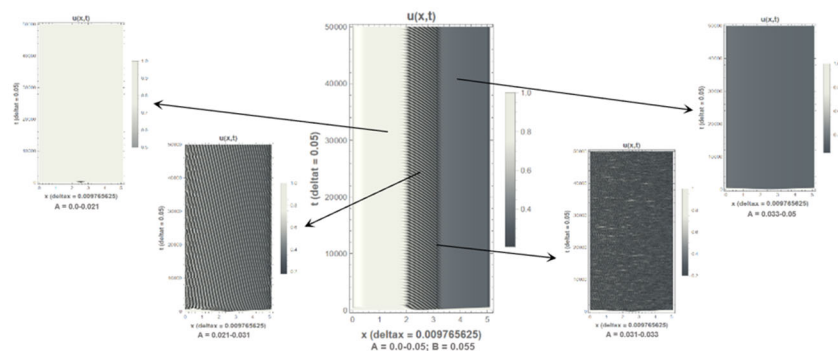
Streptomyces buecheerae sp. AC536



The Effects of Perturbations in Feed Parameters with Spatially Localized Functional Forms on Reaction-diffusion Systems

Summer Kantanen and Dr. Jason Czak
 Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

The Grey-Scott Model is a reaction-diffusion system consisting of two non-real chemical species, u and v , which react and transform with each other. Manipulation of parameter values within the model creates spatiotemporal patterns that resemble crucial biological, chemical, and physical processes, such as DNA oligomers, skin pigment development, and oscillatory chemical reactions. While extensive studies have explored these patterns using constant parameter values, this research introduces specially determined function forms to spatially vary a specified parameter. By varying system parameter values using different functional forms along the lattice, we can merge behaviors and patterns from different parameter settings within a single reaction. This innovative method not only unveils new and unique patterns but also broadens the model's applications, extending its relevance to a wider array of natural phenomena.



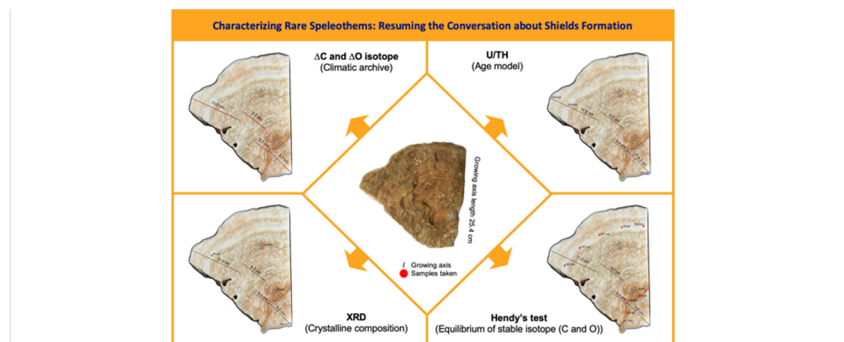
Characterizing Rare Speleothems: Resuming the Conversation about Shields Formation

Bianca P. Maldonado¹, Dr. Ángel A. García² and Dr. Ángel A. Acosta¹

¹Department of Physics-Chemistry, University of Puerto Rico at Arecibo

²Department of Geology and Environmental Science, James Madison University

In dissolution caves, there are several types of speleothems, such as stalactites, stalagmites, columns, and others. These are characteristic of the deposition of calcite through processes of water flow and dripping. Among these formations we can find the shields, alternative called discs, palettes, or plates. Unlike other speleothems, this one has not been studied, so its origin is still to question as they are not accessible or have larger quantities for intensive research. In the Shenandoah Valley, it's possible to find numerous caves with these uncommon speleothems, which allows reopening the conversation about how shields are formed. In this ongoing research, we used a shield found in Endless Caverns, located in the city of New Market, Virginia. Its dimensions are 22.3 cm long, 23.1 cm wide and 15 cm high, and 25.4 cm throughout the growing axis. For this specimen, we acquired sub samples with a resolution of 0.5 cm by micromilling following the growth axis through the concentric layers. With the sampled material, we will further several analyses including, stable isotope chemistry to find existing trends of carbon and oxygen isotopes (climatic archive), Hendy's test to detect the variation and equilibrium of stable isotope (C and O) through one layer, XRD to observe the crystallographic structure of the speleothem, and build an age model with U/Th. The objective of this research is to describe the shields in more detail to expand the knowledge about these rare speleothems.



Towards A Better Understanding Of The Relationship Between Black Hole Accretion And Maser Emission Via Mid-Infrared Variability Structure Function

Christian Orrico and Dr. Anca Constantin

Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

Accretion of matter onto supermassive black holes ubiquitously found in galaxy centers, called Active Galactic Nuclei (AGN), is an important way of identifying hidden matter in the universe. A very small fraction of galaxy centers also exhibits Microwave Amplification by Stimulated Emission of Radiation (Maser), which, when in a disc-like configuration provides a direct way of measuring two main things: 1) the mass of the black hole and 2) distances to other galaxies via a geometric method, which does not involve standard candles. Therefore, it is very important to increase the detection rates of maser discs. We can do this by better understanding the physical conditions that lead to maser emissions. There is some evidence that maser disc emission is associated with AGN. Identifying AGN emission is not a trivial matter, however variability is a good indication for this phenomenon. In this presentation we use the Structure Function as a tool to quantify the variability in Mid-Infrared emission from galaxies with and without maser emission from their centers as a novel way of connecting AGN and maser emissions.

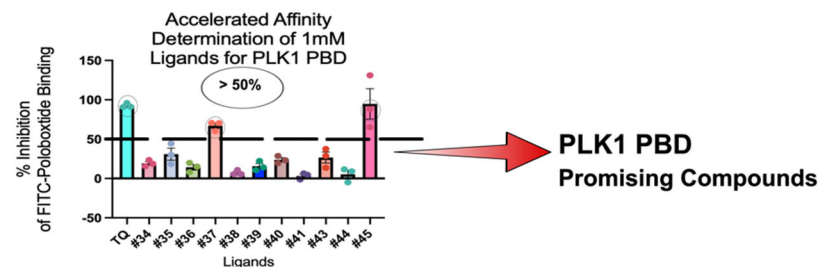
Accelerated Binding Affinity Determination using Fluorescence Polarization

Enow Otto Jr., Carter Johnson, Ashley Corcoran, and Dr. Adebowale Ogunjirin

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

School of Science, Technology, Accessibility, Mathematics, and Public Health, Gallaudet University, Washington, District of Columbia 20002

Polo-like kinase 1 (PLK1) is a key enzyme in cell cycle regulation and a promising cancer therapy target. The Polo-box Domain (PLK1 PBD) can be inhibited by binding ligands, potentially disrupting cancer cell proliferation and survival. This research investigates the binding affinity of computationally identified ligands to PLK1 PBD. Forty-six compounds were screened at 1 mM concentration using a customized fluorescence polarization protocol. The results identified six promising compounds for further investigation as potential PLK1 inhibitors.



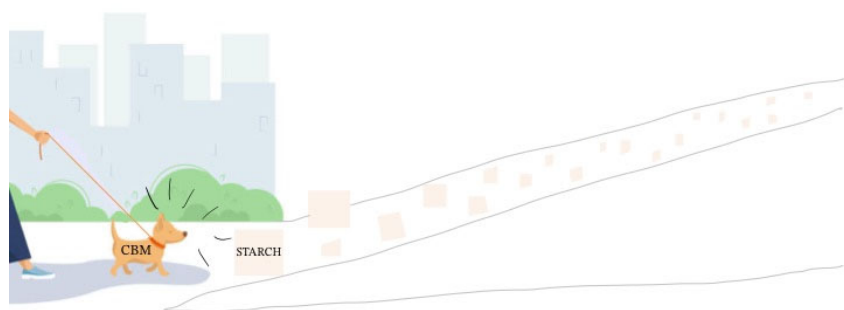
PLK1 PBD
Promising Compounds

Characteristics of Carbohydrate-binding Module of the Alpha Amylase AMY3

Ruhi Rahman and Dr. Christopher Berndsen

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

Starch is an important carbohydrate for human health, serving as a primary source of glucose that supports our bodily functions. Since humans cannot synthesize starch, we rely on dietary intake from plant-based foods. Plants regulate starch synthesis and degradation via several types of enzymes and are thought to be targeted to specific structures within starch by carbohydrate binding modules (CBMs). This targeting allows for controlled synthesis and degradation of starch. Many types of CBMs have been identified but few of them have been characterized on a biochemical and structural level. Understanding these aspects of CBMs will explain more about starch remodeling and could be useful for the development of sugar sensors. This study investigates the structural and binding properties of the carbohydrate binding module (CBM) from alpha-amylase AMY3 using small-angle X-ray scattering (SAXS) to determine its shape, and high-performance liquid chromatography with size exclusion chromatography multi-angle light scattering (HPLC SEC-MALS) to assess its size. Cross-linking experiments were performed to stabilize any CBM oligomers that form. Our findings indicate that the CBM of AMY3 forms dimers and dimerization is enhanced in the presence of long chains of glucose called maltodextrin. This comprehensive approach enhances our understanding of the AMY3 CBM's functional and structural characteristics.

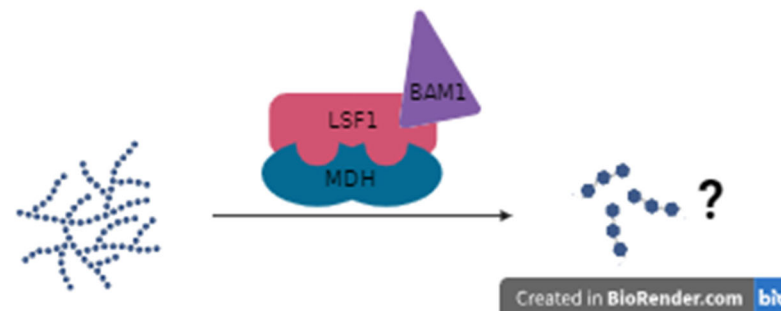


Pseudoenzyme LIKE SEX FOUR 1 Has Little Effect on Beta Amylase Hydrolysis Activity

Jackson Tester and Dr. Chris Berndsen

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

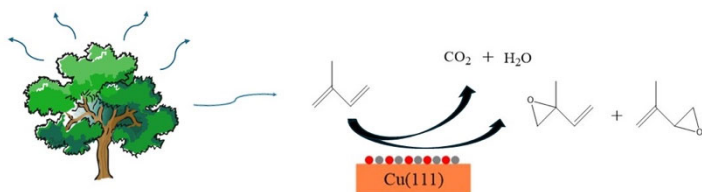
Starch degradation is vital to plant metabolism. Starch is synthesized during the day and degraded at night to sustain plant survival in the absence of sunlight. In *Arabidopsis thaliana*, hydrolase enzymes called beta amylases (BAM) play a crucial role in the degradation of starch. Malate dehydrogenase (MDH) and LIKE SEX FOUR 1 (LSF1) are two other proteins that are said to interact with BAM proteins to break down starch. The exact role of malate dehydrogenase is unknown, but certain studies suggest that it recruits BAM proteins to the starch granules themselves, initiating starch degradation. LIKE SEX FOUR 1 (LSF1) is an inactive phosphatase that may also play a role in the recruitment of BAM proteins. Previous literature suggests that a LSF1-MDH complex increases starch hydrolase activity of BAM1 3-fold compared to BAM1, LSF1, and LSF1-MDH alone. However, these studies do not use the full length LSF1 protein. Bicinchoninic acid assays (BCA) were performed to measure hydrolase activity of BAM1, as well as BAM1 coupled with a full length LSF1-MDH complex. This data suggests BAM1 by itself increases starch hydrolysis activity more than with LSF1-MDH. Future studies will incorporate other beta amylase proteins such as BAM3 and alpha amylases like AMY3 to study their effect on starch degradation activity.



Exploring the Epoxidation of Isoprene on Copper-Based Catalysts

James T. Whitted, Mollie M. Corbett, Dr. Ashleigh E. Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

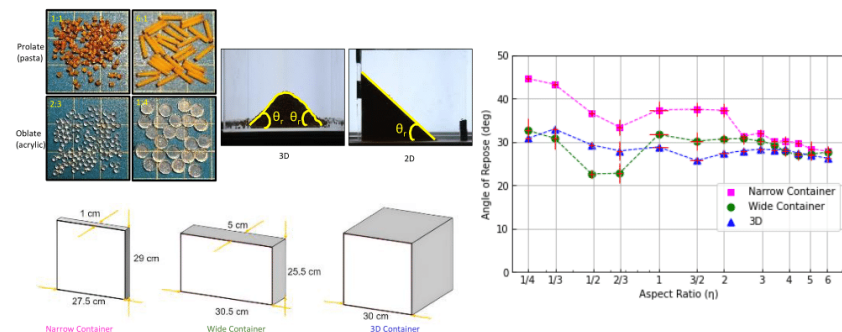
Isoprene (C_5H_8) is a common greenhouse gas that forms the infamous haze observed over the Blue Ridge Mountains. It contributes to a large portion of the planet's ozone formation, and therefore finding alternative value-added uses for isoprene is critical. Isoprene is a diene, and due to its molecular structure, has both allylic hydrogen and non-allylic hydrogen sides. It is therefore a model reactant molecule for studying selective epoxidation. Atomic oxygen on Cu(111) is known to enhance the epoxidation of propylene, which contains allylic hydrogens, while Ag(110) and Ag(111) with atomic oxygen encourages the epoxidation of ethylene, which does not have allylic hydrogens. This molecule is ideal to study epoxidation reactivity on a AgCu near surface alloy (NSA), specifically for its allylic hydrogen and non-allylic hydrogen sides, which mimic propylene and ethylene. Olefins have several different reaction pathways that can be isolated through specific reaction schemes. The major reaction pathway for isoprene is combustion. Creating an NSA comprised of Ag atoms on Cu(111) should produce a favorable surface to form an epoxide from isoprene, while also limiting the unwanted combustion pathway. Ultra-high vacuum temperature programmed desorption (UHV-TPD) spectra were gathered on clean Cu(111) and partially oxidized Cu(111) after dosing isoprene. As the amount of oxygen dosed on the surface increased, carbon dioxide yield also increased, indicating that the combustion pathway was in full effect. In an attempt to understand how our potential products would fragment inside the mass spectrometer, a mixture of 2-methyl-2-vinyloxirane and 2-(1-methylethenyl) oxirane were synthetically produced to dose into the chamber. Due to unreacted meta-Chloroperoxybenzoic acid being leftover, we refrained from dosing the low purity mixture. To minimize overoxidation of isoprene to CO_2 , Ag was deposited on Cu(111) via physical vapor deposition. Auger electron spectroscopy (AES) was used to determine Ag amounts on the surface, post-deposition. Moving forward we hope to complete multiple TPD series on the NSA and study the oxametallacycle (OMC) intermediate of isoprene using scanning tunneling microscopy (STM).



Impact of Particle Morphology, Preparation Method and Confinement on the Angle of Repose for Granular Materials

Ethan Zimmerman, Owen Paulson and Dr. Klebert Feitosa
Department Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

Understanding and predicting avalanches, mudslides, and other similar granular flows has numerous applications in geophysics, civil engineering, and mining. The angle of repose stands as a crucial parameter in characterizing particle flow within granular piles. Our investigation delves into how the angle of repose varies concerning particle aspect ratio, preparation method, and confinement. We find that the angle of repose appears independent of the aspect ratio for aspect ratios ranging from 1:4 (oblate) to 6:1 (prolate), except when under confinement, where the preparation method significantly influences the outcome. Specifically, employing a free-flowing method of pile preparation results in a decrease in the angle of repose with aspect ratio, whereas utilizing a tilting method of pile preparation leads to an increase. Wall friction and particle entanglement emerge as the most probable factors driving these observed behaviors.



STUDENT ABSTRACTS

Poster Session: Group B

Listed in alphabetical order by presenter's last name
(Student presenters underlined)

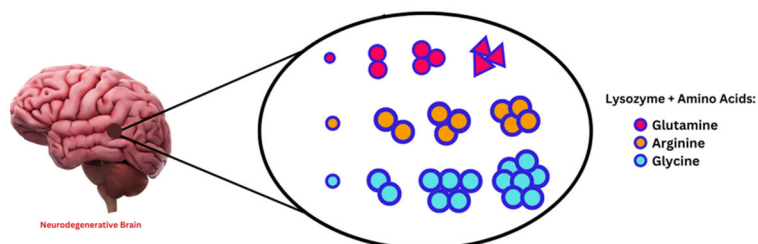
Amino Acid Influences on Lysozyme Structure, Stability, and Aggregation

Daphne M. Antwi¹, Kalany N. Santos-González¹, Dr. Gina MacDonald²

¹Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

²Department of Chemistry, University of Puerto Rico in Humacao

Neurological diseases have continued to be critical issue for many Americans. Many neurological and other diseases have unfolded, aggregated proteins that are a crucial link to uncontrolled cell death. Extensive research has demonstrated that changing the solution conditions of different proteins effects their structure, stability and aggregation. Previous studies in our lab have focused on how salts and metals influence protein stability and aggregation. Additional investigations have shown that different amino acids alter protein stability and aggregation. However, most previous studies have used heat to denature proteins and observe how their stability changes over time. This approach doesn't replicate the natural environment within cells. Current experiments in our lab are focused on how environmental conditions alter protein structure over time. This research is focused on the model protein Lysozyme and how its characteristics are affected by incubation with various amino acids. These studies have used Infrared spectroscopy (IR) and Circular Dichroism (CD) to monitor lysozyme structure, stability and aggregation. The CD results show that the presence of glutamine slightly alters protein structure after incubation while Infrared studies show that amino acids differentially influence protein aggregation.

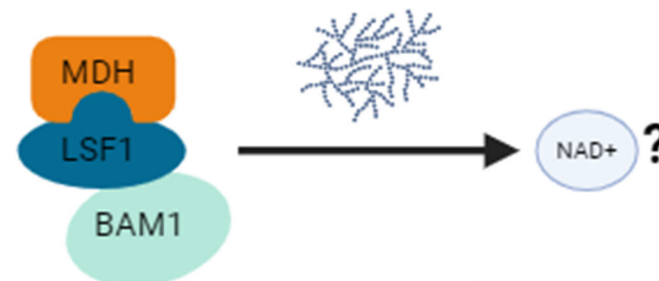


Malate Dehydrogenase and Like Sex Four 1 Activities Affected by Varying Concentrations of Starch

Trip Beaver, Dr. Chris Berndsen

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

Malate Dehydrogenase (MDH) is an enzyme that is involved in the Krebs Cycle and catalyzes the conversion of Malate to Oxaloacetate using the reduction of NAD⁺ to NADH. MDH combines with Like Sex Four One (LSF1) to recruit β -Amylases (BAMs), which break down starch. Starch has an important role in metabolism for plants as it allows them to store energy in order to survive the night. Studies suggest that when MDH and BAM combine with the pseudo-enzyme LSF1 there seems to be a 3-fold increase in starch degrading ability. The goal of this project was to test the activity of MDH while in the presence of LSF1 and BAM1 to break down NADH into NAD⁺ using Oxaloacetate. This was done using a plate reader and a 96 well plate to measure absorbance of NADH at 340 nm. Different concentrations of starch were added to the complex to determine if there was a change in the ability of MDH to convert NADH into NAD⁺. The results gathered from this project included a slight increase in MDH-LSF1 activity at lower concentrations of starch but no effect was observed at higher concentrations. Future work for this project includes adapting the protocol to be able to better read higher concentrations of starch in the plate reader without it becoming cloudy. Further work will also have to be done with Small Angle X-ray Scattering data of NAD-MDH and NADP-MDH in order to determine the structural differences and discover why they bind differently.



Optical and Microscope Characterization of Gd-doped ITO Thin Films

Trevor Brown¹, Kamryn McGary¹, David Lawrence², Costel Constantin¹ and Masoud Kaveh¹

¹Department of Physics and Astronomy, James Madison University, Harrisonburg, U.S.A.

²College of Integrated Science and Engineering, James Madison University, Harrisonburg, Virginia, U.S.A.

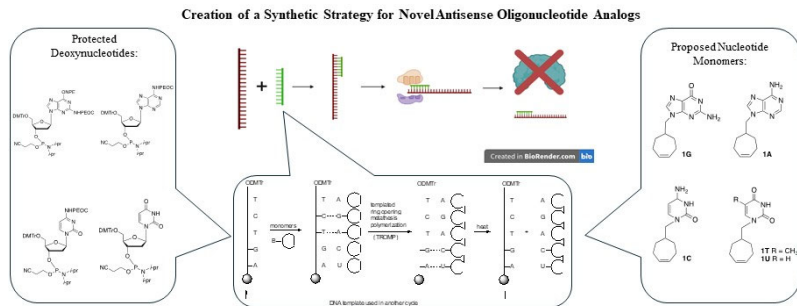
Transparent conducting oxides (TCOs) are electrically conductive, yet optically transparent due to their large energy band gap. Extensive research on these samples has led to extensive advancements in applications in energy (solar cells), optics (LEDs), and electronics (wearable gadgets). The further development of transparent conducting oxides with magnetism may lead to new magneto-opto-electronic devices, and the possibility of effectively utilizing spintronic devices, which transfer information through the propagation of particle spin rather than electron motion. This would potentially revolutionize the field of communications and computations. This study seeks to induce dilute ferromagnetism in the well-understood transparent conducting indium tin oxide (ITO) through the introduction of magnetically potent gadolinium impurities. Gadolinium-doped ITO thin films (0-24 at% Gd) were deposited using DC magnetron sputtering technique. Profilometer and scanning electron microscopy measurements were used to determine the composition of the samples and their suitability for further characterization. Optical properties of the samples were investigated using a series of temperature-dependent photoluminescence (PL) measurements. The surface morphology of the samples was determined by atomic force microscope (AFM). AFM results on the undoped ITO sample show overlapping island-like grain structures of ~5nm. The grain size appears to grow with increasing Gd concentration. PL measurements at 7K revealed an energy band gap of ~2.8 eV. Temperature dependent measurements show an increase in the PL intensity by increasing the temperature and then a decrease up to room temperature. This is tentatively attributed to band filling and then an electron hole recombination by increasing temperature.

Creation of a Synthetic Strategy for Novel Antisense Oligonucleotide Analogs

William Brown, Eric Shepard, Tengis Tamir and Dr. Debra Mohler

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

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

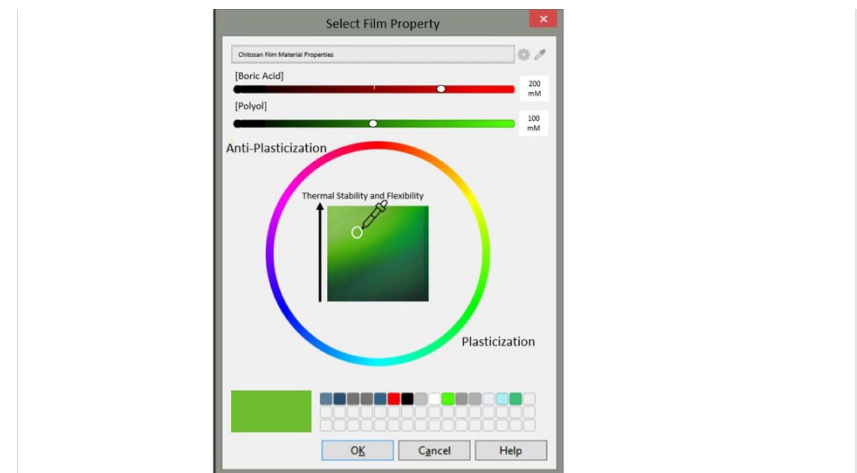


Modulating the Properties of Chitosan Films with Polyol-Boric Acid Complexes

Olivia E. Coer and Dr. Brycelyn M. Boardman

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

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

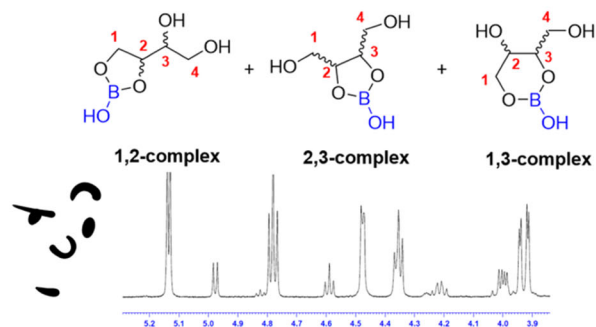


Structural Determination of Polyol-boric Acid Complexes using NMR Spectroscopy

Brandy L. Davidson and Dr. Gretchen M. Peters

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

Chitosan, a polysaccharide derived from shrimp shells, has a high propensity to form biodegradable plastics and films. Because these films are generally brittle, alcohol-rich plasticizers are often introduced to improve flexibility and mechanical properties. While chitosan materials are attractive for a variety of uses, optimizing their properties to fit a particular application is not a trivial feat. In an effort to achieve tunability in chitosan films, we theorized that the formation of complexes between the plasticizer and boric acid would alter the binding potential of the polyol and thus impact its effectiveness as a plasticizer. In particular, we anticipated that longer polyols, such as erythritol (Ery) and its stereoisomers, D- and L-threitol (Thr), would form neutral complexes with boric acid but still have the capacity to bind to chitosan. Excluding stereochemistry and the potential for dimerization, Ery/Thr can form three unique complexes in the presence of boric acid. Because these isomers are structurally quite similar, identifying and differentiating them poses a notable challenge. Here, we describe an in-depth NMR spectroscopic study into the complexation of polyols with boric acid. Simple diols were also explored in an effort to catalog observed changes in chemical shift and investigate the rate of complexation with various binding motifs. We found that the formation of boron complexes was with preferred 1,3-diols over 1,2-diols and 1,4-diols. Additionally, the complexes with terminal alkyl tails were found to form faster than those without branches, while internal tails slowed complexation. Stereochemically, we observed a preference for the D- and L-isomers of 2,3-butanediol over the meso compounds. Using these standards, we were able to determine that Ery forms the 1,3-complex as the major isomer, while D-Thr and L-Thr favor 2,3-complex with boric acid. The findings presented here provide useful insights into the role of binding motif, steric bulk, and stereochemistry on polyol-boric acid complexation. Moving forward we will investigate how the formation of neutral boron complexes with Ery/Thr alters the intermolecular interactions between glucosamine and the plasticizer.



How Effective Electrical Resistivity is as Maze Caves Form at Deeper Depths in Butler Cave

James Fuller¹, Ricky Gonzales¹, Pedro Rivera², Dr. Shane McGary¹

¹Department of Physics and Astronomy, James Madison University, Harrisonburg, Virginia, USA

²Department of Geology, Universidad de Puerto Rico at Mayagüez, Mayagüez, Puerto Rico

This research investigates the Butler Cave system, a 26.9km subsurface karst landscape discovered in 1958. Karst landscapes form when soluble carbonate rocks dissolve through the interaction with acidified water. The Butler Cave system lies along the west flank of the Sinking Creek Syncline. Much of Butler Cave is formed under the Lower Breathing Cave Sandstone and through the Devonian Tonoloway Limestone. This study utilizes Electrical Resistivity Tomography, a geophysical technique measuring subsurface apparent resistivity to create models representing the subsurface environment. These models can be interpreted to generate an understanding of the subsurface environment. However, at certain depths in the models maze cave passages merge to depict large void spaces. This issue stems from the smoothness parameter within the inversion software. The smoothness parameter penalizes high resistivity values being adjacent to lower ones. The objective of this research is to collect data from various caves in the Butler Cave area at different depths. By comparing resistivity distribution models at these depths, we aim to identify at which depths the inversion software inaccurately merges maze caves into large void spaces. This understanding will help in the future to improve the accuracy of subsurface models and the interpretation of karst environments

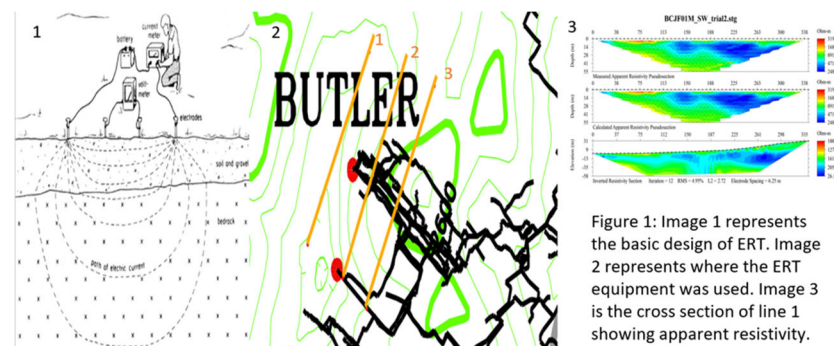
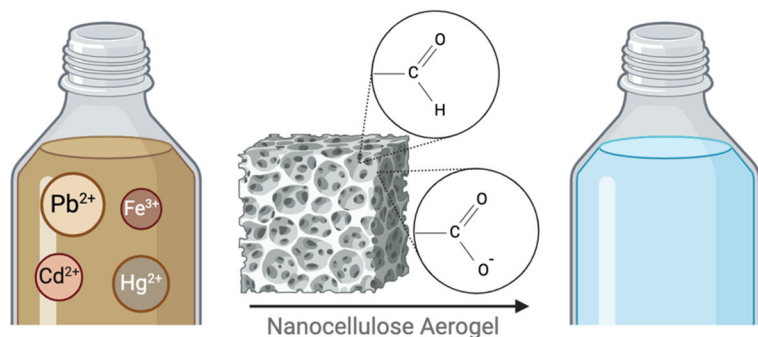


Figure 1: Image 1 represents the basic design of ERT. Image 2 represents where the ERT equipment was used. Image 3 is the cross section of line 1 showing apparent resistivity.

Exploring Nanocellulose as a Matrix for Metal Organic Framework Composites

Emma J Goehner, Stephanie J Schwender, Lewis D. Crooks IV, and Dr. Barbara Reisner
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Polymer composites containing metal organic frameworks (MOFs) are promising materials for the selective removal of metal contaminants from aqueous systems. Nanocellulose is a sustainable polymer that can be used to embed MOFs, so they do not resuspend in solution. This study explores the use of nanocellulose fibers to produce aerogels to support MOFs. Conditions were explored to make composites containing nanocellulose based ZIF-8 (Zn^{2+} and 2-methylimidazole), ZIF-67 (Co^{2+} and 2-methylimidazole), and H-KUST (Cu^{2+} and 1,3,5-benzenetricarboxylate) composites. The impact of conditions on gelation and the characterization of the materials by powder X-ray diffraction and infrared spectroscopy will be presented.



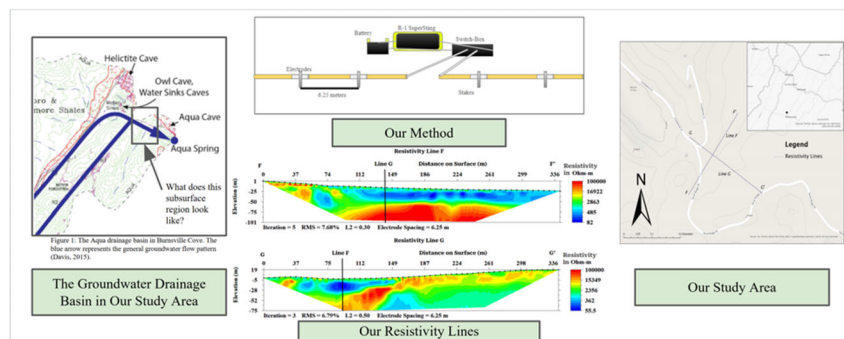
Finding Approximate Locations for Cave Systems using Electrical Currents

Ricky Gonzales¹ and R Shane McGary²

¹Department of Physics and Astronomy

²Department of Geology and Environmental Science, James Madison University, Harrisonburg, VA 22807

Electrical Resistivity Tomography is a non-intrusive geophysical detection method useful for identifying subsurface features such as groundwater conduits and void spaces. We use this method to begin constraining the extent of a recently discovered cave system in Highland County, Virginia. Our study area lies within the Burnsville Cove Region, an area with substantial karst and karst related features such as maze caves, springs, and sinkholes. In a previous project, resistivity was used to identify the subsurface path for groundwater flow through the study area. It also uncovered the existence of a previously unknown cave system along the subsurface flow path between the previously known Water Sinks and Aqua cave systems. Our work not only confirms the existence of the maze cave system but provides important constraints regarding the extent of the cave system. Additionally, the resistivity results illuminate the presence of a near-surface cave passage that might provide access to this cave system in the future.

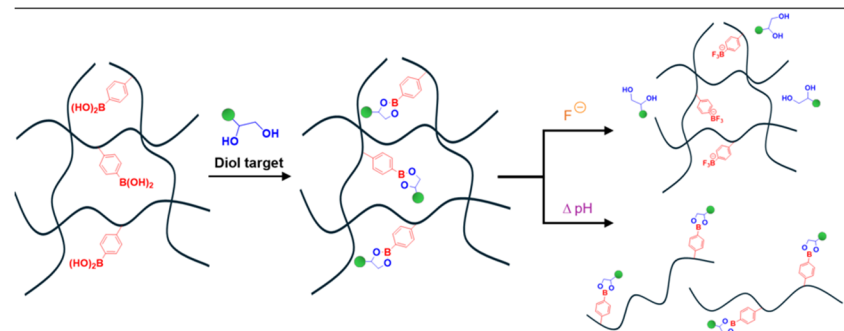


Impacts of Boronic acid on the Properties and Function of Supramolecular Peptide Gels

Anna Grove and Gretchen Peters

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

Peptide gels have been widely used for a variety of applications including drug delivery, tissue engineering, environmental remediation, and waste management. Supramolecular peptide gels are particularly attractive for these applications as they are generally non-hazardous and readily respond to external stimuli. Though largely unexplored in peptide gels, boronic acids are useful additions to soft materials; they have been shown to both induce gelation and introduce new function into gels. The work described here investigates the impact of boronic acid units on the stability and function of supramolecular peptide gels. Triphenylalanine-boronic acid (FFFBA) and other derivatives have been successfully synthesized via solid-phase peptide synthesis and fully characterized by NMR spectroscopy. In neutral pH, FFFBA readily forms stiff, self-supporting hydrogels after a heat-cool cycle. Cargo can be readily incorporated into the gel network both covalently via boronate ester formation with a diol-containing target and non-covalently via hydrogen bonding and π - π stacking with non-diols. When exposed to an external aqueous environment, the non-covalently attached cargo is rapidly expelled from the material into the surrounding solution. In contrast, diol-containing cargo remained trapped inside the hydrogel until a trigger, such as pH changes or F^- , was introduced. In the absence of a boronic acid unit, no difference was observed between diol and non-diol cargo. Notably we observed a significant difference in the rate of gel dissolution with FFFBA relative to non-boronic acid peptide gels. Thus, moving forward, we will explore the possibility of slowing and controlling the release of incorporated targets and dissolution of the material using binary mixtures. Furthermore, we will continue to evaluate the impacts of gelator structure (i.e., sequence, length, regioisomerism) on the properties and function of these materials.



Induction of Natural Products by Fungal-Fungal Co-cultures

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

Natural products—small molecules produced by plants, bacteria, and fungi that help them to secure their ecological niche—have played a major role in pharmaceutical and agrochemical development. Fungi in particular biosynthesize a variety of small molecules with a wide range of bioactivities. Natural products are produced by biosynthetic gene clusters (BGCs), which consist of one or more backbone enzymes, tailoring enzymes, and sometimes transcription factors that regulate their expression. However, the majority of fungal BGCs remain silent under laboratory conditions and their associated natural products are not produced unless induced by an external stressor. The technique of co-culturing is one such stressor, in which two or more fungal strains are grown on the same media to introduce competition for limited space and resources, ideally inducing the expression of silent BGCs that form secondary metabolites not found in monoculture. Nine fungal strains were isolated and grown from soil collected at 38°26'0" N 78°51'41" W in Harrisonburg, VA and a tenth strain was collected from Grand Caverns in Grottoes, VA. Of the 45 possible fungal-fungal co-cultures, 14 were pursued for further study due to visual changes in the appearance of the fungi in the co-culture as compared to the monoculture. Target co-cultures were prepared for chemical analysis by growing seed cultures on rice, extracting them in CHCl_3 and MeOH, and eliminating sugars and fats using liquid-liquid partitioning. The resulting extracts were dried by N_2 , following which they were analyzed using mass spectrometry-based metabolomics. Abundant chemical changes were witnessed in a subset of five co-cultures, and we are currently scaling up growth of these five co-cultures to evaluate reproducibility of BGC expression and pursue metabolites for purification. In these five co-cultures, 17 major chromatographic peaks were unique to or highly upregulated in co-culture. We have tentatively identified a subset of seven of the associated compounds using mass spectrometry and publicly available natural products databases. Two of the co-cultures have been tested in triplicate to ensure that unique chemical patterns were reproducible, and unfortunately, they did not appear to consistently produce any compounds not found in their component monocultures. Future work includes reproducing the other three co-cultures in triplicate, identifying induced compounds using existing chemical databases, and characterizing any novel compounds using ^1H NMR.



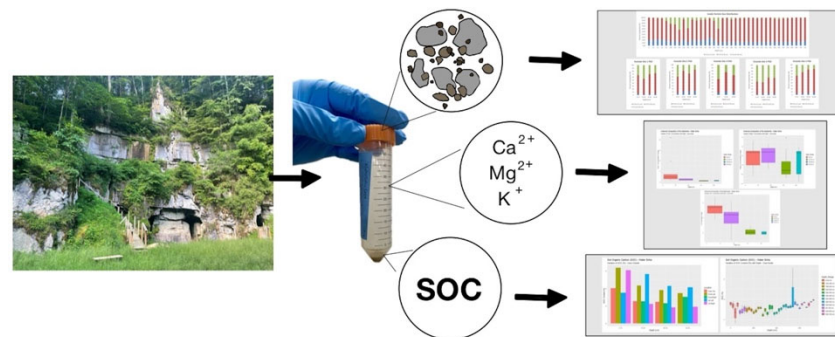
Variability of Physical and Geochemical Properties of Cave Ecosystems: A Case Study in Water Sinks Cave, Highland County, VA

Catherine Hughes¹, Dr. Dhanuska Wijesinghe²

¹Department of Environmental Engineering and Earth Science, Clemson University, Clemson, SC 29631

²Department of Geology and Environmental Science, James Madison University, Harrisonburg, VA 22807

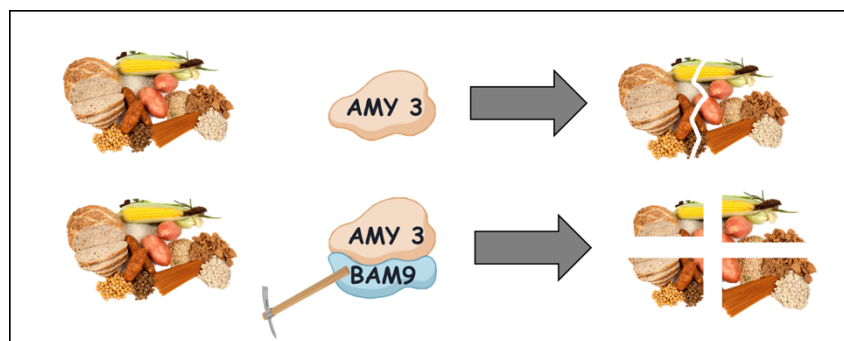
Understanding the interplay of sedimentation processes is essential to reconstructing past environments and environmental conditions and assessing ongoing ecological dynamics within cave systems. In this research, we aimed to explore the physical and geochemical properties of sediments inside Water Sinks Cave in Highland County, Virginia to reconstruct the history of these sediments and, by extension, the cave itself, focusing on whether the sediment accumulation is autochthonous or allochthonous. We collected thirty-seven sediment samples from an unstudied sediment pile in one of the upper passageways of the cave, and analyzed sediment particle size, soil organic carbon, and chemical composition. Additionally, we collected samples from five sites outside the cave for comparative analysis. Our particle size analysis revealed that most inside samples were predominately silt, with smaller amounts of clay and sand; although, variations with higher sand and lower silt content were observed at shallower depths. Outside samples were also mostly silt but had higher sand concentrations. Soil organic carbon analysis showed a slight increase in carbon levels with depth inside the cave, while outside samples exhibited decreasing carbon levels with depth. Water content in both the inside and outside samples tend to increase with depth. These findings suggest that the Water Sinks sediment pile may have resulted from multiple sediment influx periods, as indicated by similarities in particle size between the inside and outside sample groups. The soil organic carbon content of the deeper sediments within the cave supports the hypothesis that older sediments originated from outside the cave, while younger sediments may represent in situ deposits. Going forward with this project, we hope to continue work on elemental and mineral analysis as well as age dating our sediments.



Characterizing the Interaction between the Amylases BAM9 and AMY3

Luke McFather, Dr. Jon Monroe, Dr. Christopher Berndsen
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Starch is a plant polysaccharide that stores energy (carbon) for uses in biological processes such as cellular respiration and conversion into maltose. Many industries use starch, including food and beverage production, pharmaceutical companies, and construction materials. In *Arabidopsis thaliana*, there are 9 β -amylase (BAM) genes, of which 5 are catalytically active. The other 4 genes are inactive with no direct starch-degrading starch. One of these inactive amylases, BAM9, has some role in starch hydrolysis, but the specific function is unclear. Recent work in the lab has suggested a functional link between BAM9 and the alpha-amylase AMY3, but the structural and biochemical mechanism connecting these proteins is not clear. Understanding the complex mechanisms and structure of the BAM9-AMY3 interaction can lead to research development of gene modification and starch degradation implications. My research is examining the interaction between β -amylase gene 9 (BAM9) and plastid-localized α -amylase (AMY3). When paired with BAM9, AMY3 shows enhanced starch degradation activity, suggesting that BAM9 is a pseudo enzyme. It is unclear where these two proteins interact and how BAM9 stimulates AMY3 activity. To further explore the interactions between AMY3 and BAM9, we first used Fast Protein Liquid Chromatography (FPLC) to purify the AMY3, BAM9, and a series of BAM9 mutants from *E. coli*. Then we performed enzyme activity assays with wild-type BAM9 and BAM9 mutants to determine the stimulatory effects on AMY3 activity. We found that all the BAM9 mutants stimulated AMY3 activity to some degree, suggesting that these mutations did not fully interfere with AMY3 activation. Preliminary evidence suggests that W296 of BAM9 may play some role in the interaction, as assays with this mutant show a 20% decrease in stimulation. In the future, we will continue activity assays on AMY3 with new BAM9 mutants to better understand this interaction.



Fabrication of Gd Doped ITO Thin Films

Kamryn McGary¹, Trevor Brown¹, David Lawrence², Costel Constantin¹ and Masoud Kaveh¹

¹Department of Physics and Astronomy, James Madison University, Harrisonburg, U.S.A.

²College of Integrated Science and Engineering, James Madison University, Harrisonburg, Virginia, U.S.A.

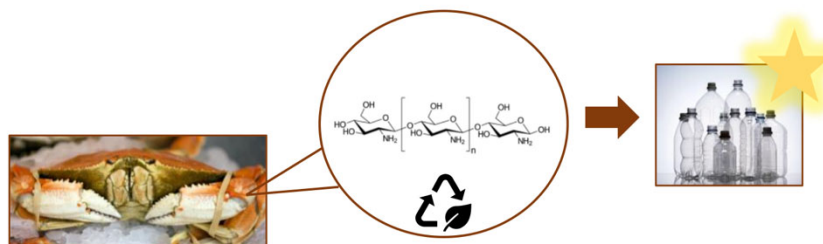
In this study, we investigate the fabrication process of thin films of Gadolinium (Gd) doped Indium Tin Oxide (ITO). ITO is a well-known transparent conducting oxide (TCO) with many optical and electrical applications. Gadolinium, a magnetically-active heavy metal, is chosen as our dopant aiming to fabricate a TCO for spintronic applications. Thin films are fabricated using DC magnetron sputtering in the JMU clean room, utilizing ITO and gadolinium targets with 7.6 cm radii. Achieving a stable plasma during the growth while varying the Gd concentration is a challenge which was overcome using aluminum disc masks of different radii inserted above the Gd target, as well as the controlling the applied DC voltage during the growth. A series of samples on silicon, sapphire, glass, and quartz substrates were grown with varying concentrations of Gd doping. The samples were analyzed with a profilometer to determine deposition thickness and edge geometry, and with a scanning electron microscope for surface morphology qualities and elemental analysis. A series of uniformly coated films were successfully grown with atomic gadolinium concentrations of 24%, 21%, 17%, 13%, and 0.05%, each with an approximate deposition thickness of 1 micrometer. There was a slight change in gadolinium percentage, approximately 1%, across the samples, with the inner and outer edges (relative to the rotating substrate platform in the sputtering device) having a higher concentration than the center. The resultant samples were deemed suitable for further characterization, and analysis for suitability as magnetic transparent semiconductor qualities. Optical characterization of these samples is presented in another work in this symposium. For future work we will be investigating their magnetic properties.

The Importance of Polyol Structure: A Spectroscopic Investigation of Triols and Linear Polyols Interaction with Glucosamine and Chitosan

Kayla H. Moore and Dr. Brycelyn M. Boardman

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

The use of bioplastics as modern alternatives to petroleum-based plastics has been a large source of interest and research in the past decade. The properties of these biomaterials are commonly developed by combining a biopolymer, such as chitosan, with a plasticizer, such as glycerol (Glyc). Our previous work involved the study of glucosamine (GlcN), the repeat unit of chitosan, with various diols to elucidate the specific binding interactions that lead to improved plasticization in chitosan films. To gain a more in-depth understanding of secondary interactions, two additional systems were investigated. The first are extended triols, specifically (1,2,4)-butanetriol (124BT), 2-(hydroxymethyl) - (1,3)-propanediol (2HMPD), and 2-(hydroxymethyl) -(1,4)-butanediol (2HMBD). Various concentrations of the triols were used to analyze how the aggregation and disaggregation of GlcN and chitosan were impacted using attenuated total-reflectance infrared spectroscopy (ATR-IR). In both molecular level and polymeric systems, the 124BT displayed the largest shift in the CN/NH and OH bend frequencies, indicative of increased hydrogen bonding, which shows the ability of the triol compound to induce aggregation and effectively plasticize. The second system investigated were the extended linear polyols, specifically, erythritol, xylitol, sorbitol, and mannitol, which contain 4, 5, and 6 alcohols respectively. Similar experiments were performed on this system. The results indicated that extending the number of alcohol units beyond 4 has no additional increase in hydrogen bonding when compared to Glyc (3-OH units). Lastly, water absorption of chitosan films containing various diols and triols were investigated. Interestingly, diols with 1,3 binding absorb ~2 times their mass in water, where 1,2 binding diols absorb ~4-6 times their mass. This absorption happens within 1 hour and remains constant up to three hours. Conversely, 124BT and Glyc absorb relatively small amounts of water, 0.2-0.9 times their mass over a 3-hour period, whereas 2HMPD and 2HMBD continue to absorb water over time with a maximum of 9 times their mass. These results highlight the importance of both primary and secondary binding interactions with respect to plasticization efficiency.



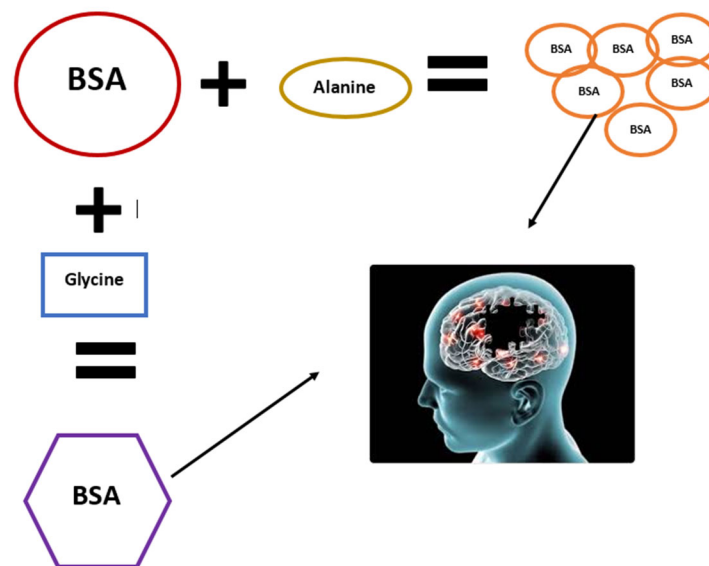
Circular Dichroism and Infrared studies of Amino acid influences on Bovine Serum Albumin Structure and Aggregation

Estrella Rayner¹, Carson Wilkinson² and Gina MacDonald²

¹Department of Science and Mathematics, Rochester Institute of Technology/National Technical Institute for the Deaf, Rochester, NY 14623

²Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

The misfolding of proteins is linked to many neurological diseases. The presence of salts and different metal ions are known to influence protein stability. The protein Bovine Serum Albumin or BSA, is a model protein that has been used in numerous studies. Previous studies have shown that amino acids such as arginine, glutamine and histidine alter the structure and aggregation of proteins. These studies used Circular Dichroism (CD) and Infrared spectroscopy (IR) to study how different amino acids effect proteins after incubation over extended periods of time. The structure and aggregation of the proteins will be monitored over time to determine how various amino acids such as: arginine, glutamine, histidine, aspartic acid, glycine and alanine alter BSA structure and aggregation at pH 7.5. Initial studies reveal that alanine may cause slight changes in aggregation and glycine may alter the stability of BSA after incubation at room temperature.



Analysis of Cave Sediments and Morphological Controls on Deposition, Butler Cave, Burnsville Cove, Virginia

Pedro Rivera¹, Bryan Crowell², Dr. Dhanuska Wijesinghe³ and Dr. Shane Mc.Gary⁴

¹Department of Geology, Universidad de Puerto Rico at Mayagüez, Mayagüez, Puerto Rico

²Department of Geology and Environmental Science, James Madison University, Harrisonburg, VA 22807

The arrangement of passages and halls found in Butler Cave located in Bath County, Burnsville Cove, Virginia raise intriguing questions about the nature of its formation processes. While most of its passages appear to be formed by epigenetic influence, sedimentation and geometry of some passages point out that a mixture of both epigenetic and hypogenic processes might have been responsible of their formation. The morphology of these passages changes periodically throughout the whole geologic expansion of the cave, as we move further downstream these passages widen into large halls and narrow down to canyon like passages. This study aims to analyze the physical sedimentological properties of deposits found across five collection sites to describe changes throughout an area of eccentric morphology. These sedimentological properties could contribute to further understanding of the evolution of Butler Cave's drainage patterns and hydrogeological cycles. The study area selected for research purposes is concentrated on a section of the cave that encompasses the Silt Crawl, Dry Sumps, Showers, and the French Passage. Particle sizes were characterized using a Laser Diffraction Particle Size Analyzer to describe size distribution across each of the sections at different depths. Additionally, total organic carbon content was quantified for each of the samples employing the Loss of Ignition method. On field morphological observations and sedimentological data, along with relevant data from earlier studies, reveals a karst conduit paleo-flow arrangement derived from overflow and constricted drainage passages of the Sinking Creek waters. Further research should focus on analyzing the morphological characteristics of Butler Cave on a greater scale from a hypogenic standpoint, with the intention of differentiating its stages of formation through geologic history.



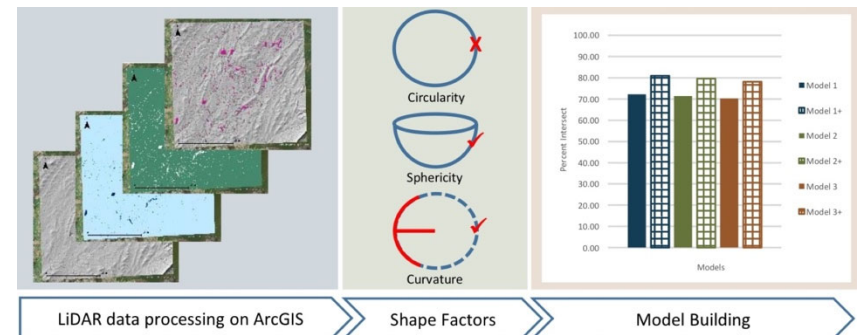
Automated Sinkhole Mapping with ArcGIS Using Shape Factors in Harrisonburg, VA

Cadence Russell¹, Dr. Yonathan Admassu² and Dr. Dhanuska Wijesinghe²

¹Department of Natural Sciences, Daemen University, Amherst, NY 14226

²Department of Geology and Environmental Science, James Madison University, Harrisonburg, VA 22807

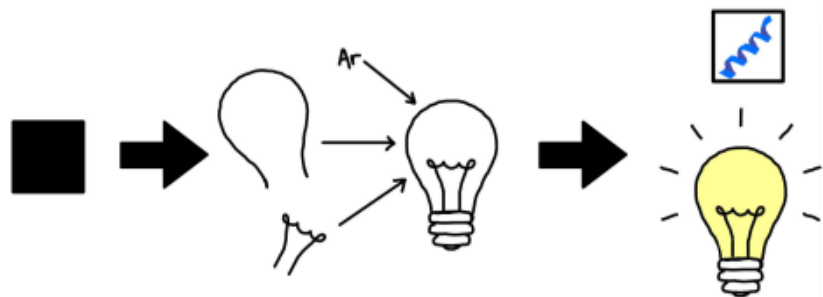
Sinkholes are common features in karstic environments that pose threats to infrastructure and serve as conduits for potential groundwater pollution. Mapping sinkhole occurrence and potential formation is critical for hazard assessment, but traditional methods through visual identification are ineffective and inefficient. The objective of this study is to test the effectiveness of automated sinkhole mapping and develop models for further implementation. An approximately 15000 m x 15000 m study area encompassing Harrisonburg, VA was chosen for this study, with control sinkhole data sourced from VA Energy and 1 m LiDAR from the USGS. High-resolution digital elevation models (DEMs) generated from LiDAR in ArcGIS make processing closed depressions in a landscape simple, but returns too much noise. Using methodology adapted from Admassu & Woodruff (2021), DEMs were processed to isolate depression polygons and generate shape factors. Differentiating between sinkholes and non-sinkholes using shape factors such as circularity, sphericity, and curvature through linear discriminant analysis returns success rates of ~71%, with maximum curvature found to be the most efficient variable separating sinkholes from non-sinkholes. Additionally, all models identified sinkholes not originally mapped in the control. Future work should be concentrated on the potential difference in effectiveness in automated sinkhole mapping between urban, suburban, and rural landscapes.



Development of a Colorimetric Assay to Test Amylase Activity

Sara E. Scanlan, Dr. Jonathan D. Monroe and Dr. Christopher E. Berndsen
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Starch is the primary form of energy storage for plants. During the day, starch is synthesized, stored, and then broken down in the chloroplast during the night to generate usable sugar in the form of maltose. Among the enzymes that catalyze this degradation are β -amylases, which cleave two glucose units from the non-reducing end of a polyglucan chain, forming β -maltose. The Arabidopsis β -amylase (BAM) gene family is commonly used as a model system to study amylases. β -amylase (BAM) proteins are diverse in both structure and function, and collectively contribute to a number of cellular processes including gene expression and starch metabolism in plants. There are five catalytically active BAMs in Arabidopsis that are expressed under different conditions and are localized either in the chloroplast or the cytoplasm, although their specific functions are unclear. In order to investigate the enzyme kinetics of the five catalytically active BAMs, a modified BCA assay was used. The BCA assay works through reduction, and since the substrates of β -amylases are reducing sugars, the assay can be used to quantify the change in concentration of reducing sugars and therefore the amount of product generated. The assay method was validated using a well characterized ortholog found in sweet potatoes (*Ipomoea batatas* BAM5) and tested using multiple substrates, including soluble starch and maltodextrins of varying length. The validated assay can be used to investigate the kinetics of the five catalytically active BAMs, ultimately leading to a comprehensive understanding of the way different Arabidopsis β -amylases interact with substrates and function within the plant.



STUDENT ABSTRACTS

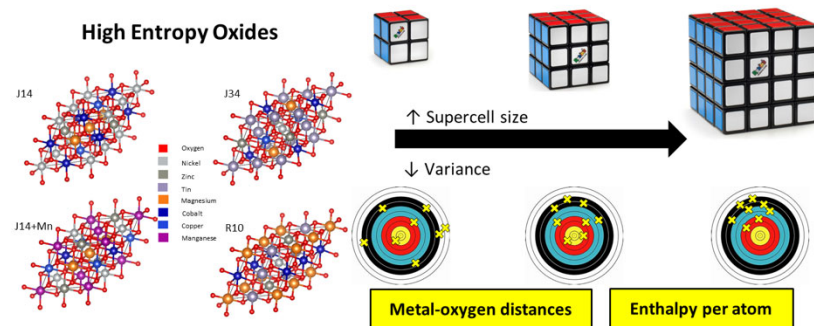
Multi-Slide Presentations: Session II

(Student presenters underlined)

Computational Investigation of High Entropy Oxides

Grace Chamberlain, Lily Jade Joyce, and Dr. Kendra Letchworth-Weaver
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

High entropy oxides have the potential to improve lithium-ion batteries, thermoelectric materials, and corrosion shielding, but synthesizing novel compositions of high entropy oxides can be time-consuming and expensive due to their high formation temperatures. High entropy oxides are characterized by long-range order in the lattice structure, with minimal movement of the metal atoms away from their ideal positions, but short-range chemical disorder leading to significant distortion of the metal-oxygen bonds from one local environment to another. Using high-performance computing (HPC) resources at James Madison University, the University of Virginia, and Argonne National Laboratory, we can run JDFTx, a density-functional theory (DFT) software, to model high entropy oxides and collect statistical data on their bond lengths and enthalpies of formation. By increasing the supercell size used in the DFT calculation we can increase the number of metal atoms per unit cell and therefore the length scale for sampling configurational disorder. Our DFT calculations determined that larger supercells produce the most enthalpically favorable results and the results which best align with available experimental data for formation temperature. Our results will be used to train a machine learning model to identify promising compositions of novel high entropy oxides, potentially allowing for more efficient, cost-effective synthesis of high entropy oxides.

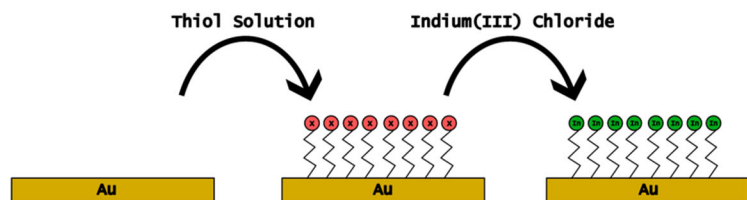


Indium Modification of Self-Assembled Monolayers

Stephan Simons and Dr. Chris Hughes

Department of Physics, James Madison University, Harrisonburg, VA 22807

Self-Assembled Monolayers (SAMs) are spontaneously formed chains of organic molecules that create a surface coating, changing the wetting, adhesion, and chemical resistance from the original surface. SAMs on gold face many challenges, as any imperfection in the gold surface or solution will impact the quality of the monolayer. A SAM with an Indium metal functional group may be used to emit gamma rays to be used in medicinal applications further down the line. So far, we have established methods for creating clean SAMs that interact with Indium(III) Chloride to potentially deposit the surface needed.



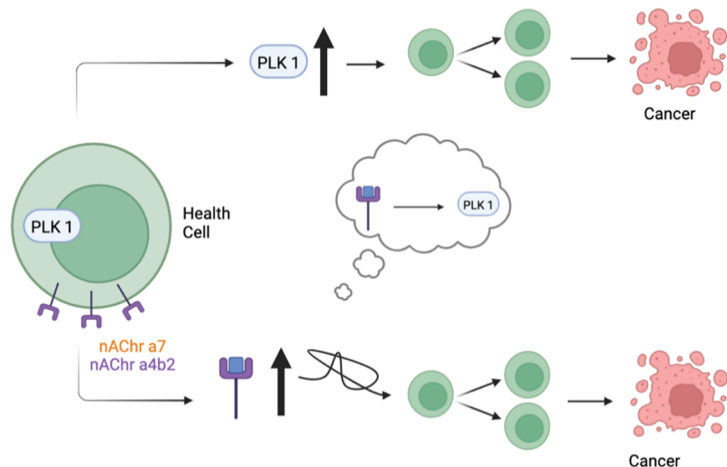
Synthesizing Nicotinic Analogue to Inhibit PLK 1 PBD

Kyle Shipman and Dr. Adebawale Ogunjirin

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

Department of Science, Technology & Mathematics, Gallaudet University

Polo Like kinase 1 (PLK1) is a crucial regulator of cell cycle progression and a promising target for cancer therapy. The Polo-box domain (PBD) of PLK 1 plays a pivotal role in its localization and substrate recognition. Here, we propose a novel approach to inhibit PLK1 PBD using a synthesized nicotinic analogue. Inspired by the structural features of nicotine compounds and its derivatives, our analogue is designed to competitively bind to the PBD, thereby disrupting PLK1 function. This study outlines the rational design, chemical synthesis, and preliminary biological evaluation of the nicotinic analogue.

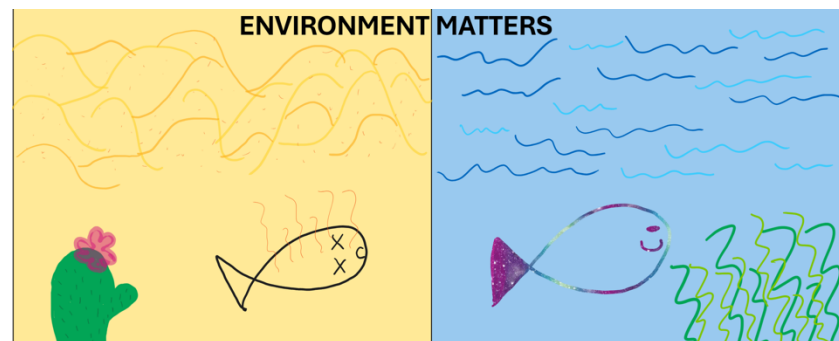


Environmental Effects on the Mechanism of Starch Cleavage in beta-amylases

Angelina M. Sardelli, Dr. Christopher E. Berndsen

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

Plant starch, a polysaccharide glucose chain, makes up part of the global food supply chain. The beta-amylase (BAM) family is a group of enzymes that catalyze the degradation of starch in plants. There are nine BAMs: five catalytically active (BAM1, BAM2, BAM3, BAM5, and BAM6) and four catalytically inactive (BAM4, BAM7, BAM8, and BAM9). We focused on two of the active BAMs, beta-amylase 5 (BAM5) and beta-amylase 3 (BAM3). Interestingly, the active site residues are largely conserved in the BAM family, and especially between BAM5 and BAM3. However, each of these BAMs have varying catalytic activities and specificities when exposed to starch. The current proposed direct attack mechanism for BAMs is unable to explain this finding. It is possible that the rate of catalysis in different BAMs is affected by differences in the active site environments of each of the BAMs. In order to study these potentially different environments and the effects on the mechanism, we performed molecular dynamics simulations on BAM3 and BAM5 and compared the enzyme dynamics and chemical properties. Quantum Mechanics/Molecular Modeling simulation suggested the geometry for an associative transition-state for BAM5. We then compared models of BAM5 and BAM3 in the apo, substrate-bound, product-bound, and transition state-mimic bound forms. After performing a series of OpenMM simulations, we analyzed the differences in calculated RMSF and pKa. Both BAM3 and BAM5 were predicted to have significant shifts in the RMSF and pKa values of their active site residues over their respective simulations. As the active site shifts in BAM3 and BAM5 were similar to each other, we hypothesize that their mechanisms of action are similar as well. In the future we will continue to observe how active site environment leads to different substrate specificity and catalytic activity in the remaining seven BAMs.



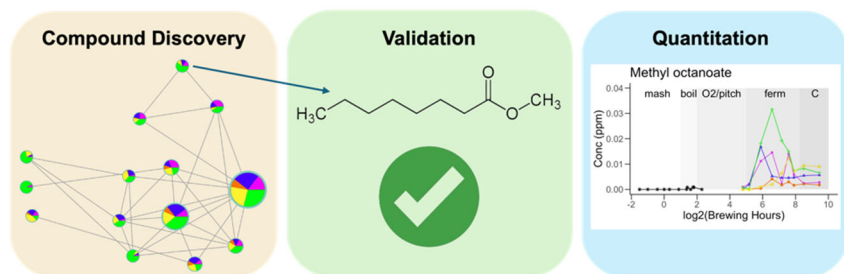
Identification, Validation, and Quantitation of New Flavor Compounds in Single Malt, Single Hop (SMaSH) Beer using Molecular Networking

Katelyn Bowers, Dylan Virts, and Dr. Christine Hughey

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

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

Beers brewed : Belgian Saison, California, English, Extreme Fermentation, Cech Pilsner



STUDENT ABSTRACTS Multi-Slide Presentations: Session III

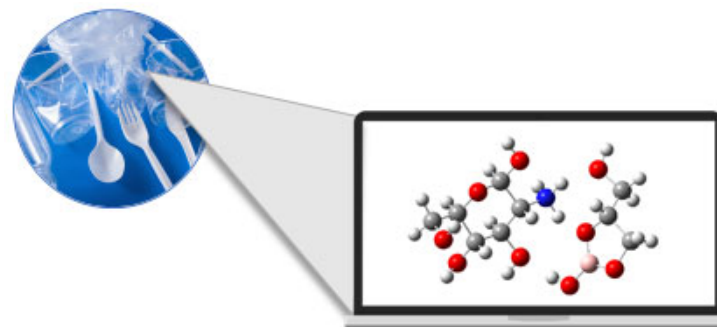
(Student presenters underlined)

Glycerol Boric Acids Interacting with Glucosamine

Elaina X. Manyin and Dr. Isaiah Sumner

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

Plastic pollution has been a growing problem around the globe for many reasons including increased environmental waste, harm to animals, and health and environmental issues. One big problem with current plastic is the material does not biodegrade. To create a more environmentally friendly plastic, chitosan, which comes from crustaceans' shells is combined with plasticizers to create biodegradable plastics. In a recent set of experiments, borate esters with glycerol were used as plasticizers, which resulted in poor plasticity. However, borate ester plastics are stiffer and have a greater thermal stability. In order to understand the molecular interactions that lead to the plastic's properties, computational experiments were run to examine the interactions between β -D-glucosamine (the repeat unit of chitosan) and glycerol boric acids (1,2-glycerol boric acid or 1,3-glycerol boric acid). Different geometries of glucosamine/boric acid complexes were optimized, and vibrational frequencies were calculated at the M06-2X/6-311+G(2d, p) level of theory. Results showed that 1,2-glycerol boric acid interacts more strongly with glucosamine than 1,3-glycerol boric acid. Furthermore, important IR stretches were identified to assist in experimental IR analysis. Specifically, the H-N-H stretches around 1620-1680 cm^{-1} , B-O stretches (1000-1500 cm^{-1}), B-O-H stretch (995-1300 cm^{-1}), and out of plane boron stretch (600-700 cm^{-1}) are clear, identifying peaks. Finally, ΔG s of reaction for the formation of the borate esters (1,2-glycerol boric acid, 1,3-glycerol boric acid, 1,2-propanediol boric acid, and 1,3-propanediol boric acid) from boric acid and different polyols were calculated. These calculations explain experimental data, which show an equal amount of 1,2- and 1,3- glycerol boric acid is made and more 1,3-propanediol boric acid is made than 1,2-propanediol boric acid.



Building and testing a Cosmic Ray Telescope for Micro-Pattern Gas Detector characterization

James Love, Jr, Mikayla Picardo, Aidan Pizarcik, Dr. Gabriel Niculescu, and Dr. Ioana Niculescu
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

Micro Pattern Gas Detectors (MPGDs) are modern-day detectors used in experimental nuclear and particle physics. The passage of subatomic particles is detected via gas ionization and electron amplification, with good time (~ns) and position (~tens of microns) resolution. As the JMU nuclear physics group is instrumenting a laboratory dedicated to MPGD characterization, we constructed a cosmic ray telescope consisting of two scintillator paddles. These will define the trajectory of a cosmic ray muon and their coincidence signal will provide the trigger for an MPGD prototype. Here we report on the mechanical design and construction of the stand, and present results from initial test runs.

A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs

Eric J Shepard, Tengis Tamir, and Dr. Debra Mohler

Antisense oligonucleotide analogs (ASOs) are short, modified RNA molecules that have the ability to bind messenger RNA (mRNA) and prevent protein transcription through various mechanisms. ASO technology has the potential to prevent or reduce the severity of numerous diseases by limiting harmful protein production. In vivo, ASOs often face degradation, membrane impermeability, RNase activity, and non-specific activities. In an effort to address these challenges, we propose to produce more stable ASO analogs via a novel synthetic strategy from nucleoside analogs. The synthesis and characterization of the Adenine, Cytosine, Guanine, Thymine, and Uracil derivatives have all been achieved.

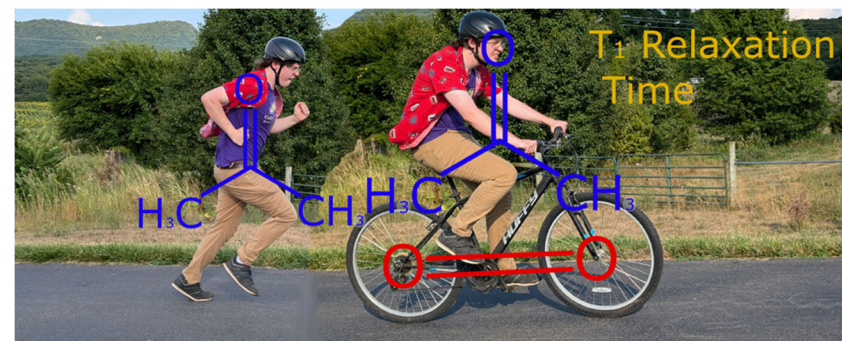
In order to polymerize the nucleic acid derivatives into the ASO analog, a reusable oligonucleotide template on a solid support is needed. Therefore, our current work is focused on modifying the protecting group strategy by which oligonucleotide strands are synthesized on the solid support. The protection of 2' Deoxyadenosine has been achieved, while the protection of 2' Deoxycytidine, 2' Deoxyuridine, 2' Deoxyguanosine are still ongoing.

Acetone's abnormal relaxation time trend is a result of dissolved oxygen

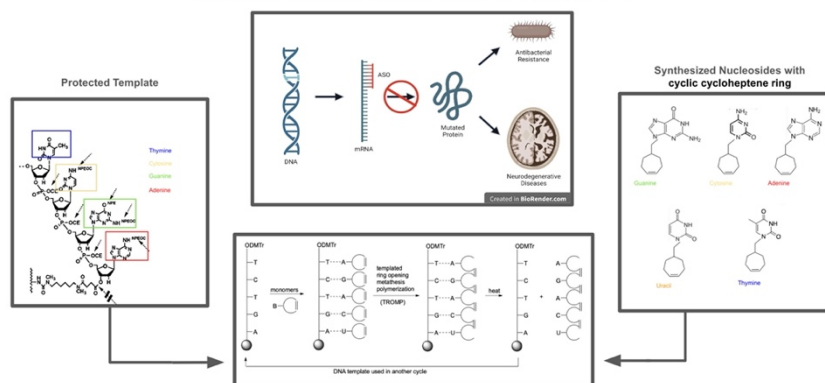
Patrick T. Randolph and Dr. Thomas C. DeVore

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

It has long been known that adding paramagnetic substances to a solution will change the observed chemical shifts and T1 relaxation times. Since molecular oxygen is paramagnetic, all NMR of molecules obtained in air will be influenced by this paramagnetic species. The effect of oxygen on NMR is most apparent for the NMR spectra of vapor species in air. For example, in methanol, the $\delta(\text{CH}_3)$ moves from 4.0325 ppm for the neat liquid to 6.1430 ppm for the vapor in air and the T1 decreases from 4.034s to 426.8ms. Since the concentration of air dissolved in most NMR solvents is low, the effect oxygen has on solvent state NMR is largely ignored. We have found that there is enough oxygen dissolved in acetone and acetonitrile to have a significant impact on the NMR spectra. Small concentrations of both solvents in DCCl_4 had chemical shifts of 2.1764 and 1.9864 ppm and T1 relaxation times of 5.879s and 4.763s respectively. The T1 observed for the neat liquids were much faster at 44.54ms and 157.3ms and had chemical shifts of 3.0080 ppm and 2.7162 ppm respectively.



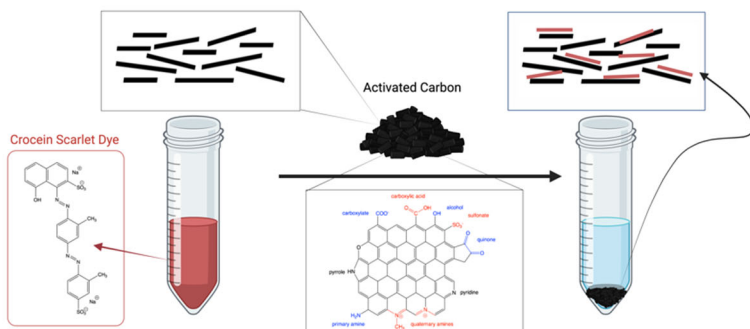
A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs
Tengis Tamir, Eric Shepard, Rhody Brown and Dr. Debra Mohler
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807



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

Emma J. Goehner, Stephanie J. Schwender, Lewis D. Crooks IV, and Dr. Barbara Reisner
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

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



Coupling between X-Ray obscuration and UV absorption by AGN accretion disk winds

Jakeline Veliz Diaz and Dr. Keigo Fukumura
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

In this experiment we aim to construct a theoretical model that can account for the observed correlation between X-ray obscuration (From *Chandra* X-ray data) and UV absorption (From *Hubble* space telescope) due to CIV transition. In the context of magnetically driven disk wind scenarios, we calculate the broad band AGN spectrum through photoionization processes for various wind parameters; e.g. Wind number density ($5.9e12 - 1.7e14 \text{ cm}^{-3}$) and radial density profile ($n \sim r^{-0.7-1.2}$). These calculations will help us constrain the wind structure in an obscured AGN environment. So far, we've seen that the predicted correlations appear to be independent of these parameters.

We gratefully acknowledge these funding sources for generous support of student research:

National Science Foundation, including the following grants:

- REU : CHE-2150091
- REU : EAR-2050819
- RUI : PHY-1614475, MCB-1817448, AST-1814594, MCB-1607024, MCB-1616467, MCB-2322867

4-VA

ACS Petroleum Research Fund, including the following grant: 59504-UR4

American Society of Plant Biologists

Argonne National Lab

Camille and Henry Dreyfus Foundation

Department of Defense – ASSURE

Department of Energy – Office of Science

International Society for Chemical Ecology

Jeffress Memorial Trust

JMU Second Century Scholarship

JMU/CSM Summer Scholarship Stimulus Program

NASA/XGS grant 80NSSC23K1021

Research Corporation for Scientific Advancement

Thomas F. Jeffress and Kate Miller Jeffress Memorial Trust

Tickle Summer Research Scholarship

JMU College of Science and Mathematics

JMU Center for Genome and Metagenome Studies

JMU Center for Materials Science

JMU Department of Chemistry and Biochemistry

JMU Department of Mathematics and Statistics

JMU Department of Physics and Astronomy

James Madison Innovations, Inc.

The Madison Trust—Fostering Innovation and Strategic Philanthropy

