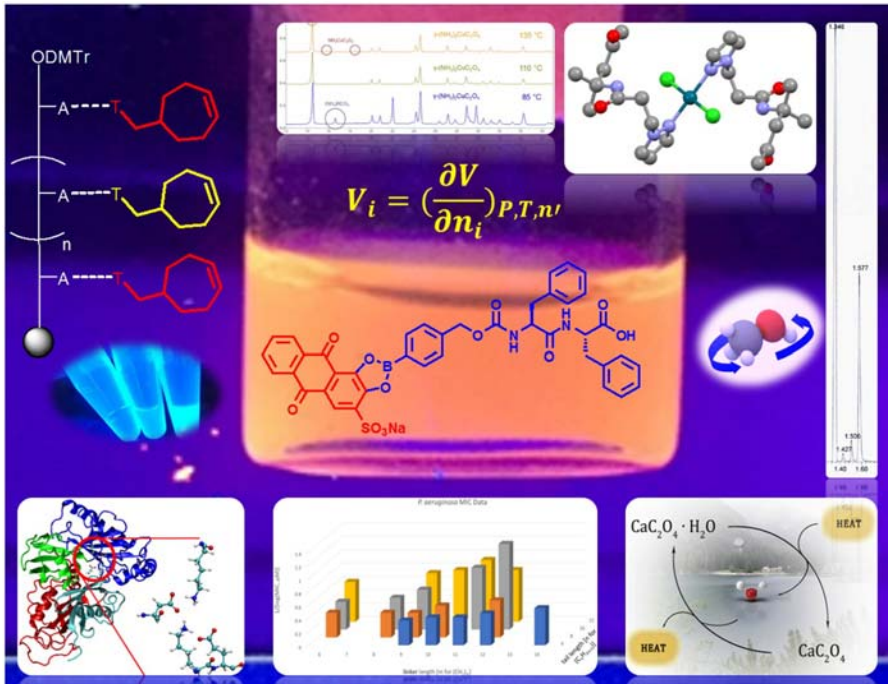
JAMES MADISON UNIVERSITY®

**DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**




# 44TH ANNUAL SPRING UNDERGRADUATE RESEARCH SYMPOSIUM

## THURSDAY APRIL 11, 2019

ORAL SESSION I: 3:00 – 4:00 PM (FESTIVAL HIGHLANDS)
POSTER SESSION: 4:15 – 5:15 PM (PCB LOBBY)

## FRIDAY APRIL 12, 2019

ORAL SESSION II: 1:30 – 3:15 PM (FESTIVAL HIGHLANDS)
SPECIAL ANNOUNCEMENTS: 3:40PM (ISAT 159)
KEYNOTE ADDRESS: 3:45 – 4:45 PM (ISAT 159)

*See back cover for image description.*

44th Annual Department of Chemistry and Biochemistry
Spring Undergraduate Research Symposium

## Keynote Speaker

**Lisa M. Christianson, MD, MPH**
**(JMU Class of 1995)**
*University of Virginia Student Health Center*
*University of Virginia School of Medicine*
Charlottesville VA

Dr. Christianson received her BS in Chemistry in 1995, with a minor in French. She received her MD from the University of Virginia School of Medicine in 1999, and continued at UVA for a residency in Obstetrics and Gynecology, completed in 2003. After completing residency, she worked in private practice, before returning to UVA to complete a Masters in Public Health degree in 2005. During this time she also began working at the UVA Student Health Center. After some additional time as a private practice Ob/Gyn, she attended the University of North Carolina Chapel Hill for a residency in Preventive Medicine, with a concentration in General Preventive Medicine and Public Health. After this, Dr. Christianson returned to UVA Student Health, and has been there ever since, serving the gynecology needs of the UVA students, and also directing the fourth year clinical elective in ambulatory gynecology at Student Health. Her special interests include polycystic ovary syndrome and other endocrine issues, vulvar pain and other chronic pain syndromes, long-acting reversible contraception, and prevention of chronic diseases. Her very special love is teaching – medical students, patients, colleagues, or anyone who will listen. Dr. Christianson also works for the UVA School of Medicine as a coach for the Foundations of Clinical Medicine course, which teaches medical students the art and science of taking a history, performing physical examinations, developing clinical reasoning skills, and communication, as well as general development as a health professional. She lives in Charlottesville with her husband, two daughters, and two cats.

## Past Keynote Speakers

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

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

| **Oral Session I: Thursday April 11, 2019 *(Festival Highlands)*** | | |
|---|---|---|
| **3:00 pm** | Maria DePonte, David Boyle, Jeremy Wilke, Maxwell Z. Gillum, Hasan Kaleem, Daniel A. Schossler and Dr. Ashleigh E. Baber | The Effect of Varied $TiO_2$ Coverages/Au(111) on Ethanol Selectivity |
| **3:15 pm** | Katherine L Elliott, N. Cole Seward, Heath Hampton and Dr. Isaiah Sumner | Study of the Lysine Deprotonation Mechanism in Ubiquitin Conjugating Enzyme, Ubc13 |
| **3:30 pm** | Tabitha J. Hain, Dr. Barbara A. Reisner, and Dr. Thomas C. DeVore | Investigation of the Ammine-Copper-Oxalate System |
| **3:45 pm** | Masha Pozhilenko, Will Vakay and Dr. Yanjie Zhang | Partial Molar Volumes and Volume of Mixing of Salts and Osmolytes |

(Student presenters underlined)

| Poster Session: Thursday April 11, 2018, 4:15 – 5:15 pm *(PCB lobby)* | |
|---|---|
| Avery York, Kevin Dannaher and Dr. Gretchen Marie Peters | Design an Synthesis of Dipeptide-Boronic Acid Gelators |
| Adrianne D. Lee and Christopher E. Berndsen | The Structure and Functional Characterization of the *Leishmania donovani Ufm*-ylation Pathway |
| Benjamin W. Adams and Dr. Nathan T. Wright | Purification and Characterization of the E. Coli Common Pilus Protein EcpD |
| Sara Hildebrand, Dr. Donna S. Amenta and Dr. John W. Gilje | Synthesis and Characterization of Palladium(II) Complexes with Substituted N-Pyrazolylpropanamide and N-Trizaolylpropanamide Derivatives |
| Kendahl L. Ott, Taylor L. Albertelli, Heather Manring, Stuart Campbell, Maegen Ackermann and Dr. Nathan T. Wright | Towards the inhibition of calpain-dependent desmoplakin cleavage in arrhythmogenic cardiomyopathies |
| Dean R. Kedir and Dr. Linette M. Watkins | Kinetic Studies of 2-(2'-hydroxyphenyl)benzenesulfinate desulfinase substrate analogs |
| Brenden K. Wimbish, Elizabeth Terry, Kyle Seifert and Dr. Kevin L. Caran | Colloidal and Antibacterial Studies of Novel Polycationic Amphiphilic Polymers |
| Chunyi Guo, Erika Hutchinson and Dr. D. M. Downey | Pitt Springs Run: A Tale of Two Water Chemistries |
| Samuel D. Fontaine, Coleman M. Swaim , P. Raj. Pokkuluri and Dr. Oleksandr Kokhan | Engineering a Cytochrome with a Tunable Bandgap Potential |
| Maxwell Z. Gillum, Jeremy A. Wilke, Maria C. DePonte, Eric M. Maxwell, Daniel S. Schlosser and Dr. Ashleigh E. Baber | Olefin Desorption Studies on Au(111)-Based Catalysts |
| Madison A. Roberts Chunyi Guo, Michael E. Petit and Dr. Daniel M. Downey | LAKE KEOKEE: Physical -- Chemical Parameters, Fish Populations and Management Issues |
| Tyler M. Miller, Emma Putnam, Adam McLuckie, Michael Khafaji Zadeh, Justin Nguyen and Dr. Kevin L. Caran | Synthesis and Antibacterial Study of Tetracationic Amphiphiles |
| Tyler Brittain, Matt O' Malley and Dr. Oleksandr Kokhan | Expression and Preliminary Characterization of GSU0105 |
| Daniel M. Paunovic and Dr. Barbara A. Reisner | Using COPUS to Inform Teaching in Foundation Inorganic Chemistry Courses |
| Nicholas J. Valle and Dr. Debra Mohler | Two synthetic approaches in the formation of a guanosine analog: connecting 2-amino-6-chloropurine to a novel 7-membered cyclic alkene alcohol. |
| Dariia Yehorova and Dr. Brycelyn M.Boardman | Investigation of donor/accepter properties of a fluorene based small molecule for flexible solar cell applications |
| Daniel A. Schlosser, Jordon S. Baker, Hasan Kaleem, Maxwell Z. Gillum, Maria C. dePonte, Eric M. Maxwell, Catherine Dukes and Dr. Ashleigh E. Baber | Surface Characterization of Ethanol Desorption from Silver 111 Defective Sites |
| Nithesh P Chandrasekharan, Ian R. Roy, Jonathan D Monroe PhD and Dr. Christopher E. Berndsen | SAXS and MD studies on β-amylase 2 tetramer in Arabidopsis thaliana |
| Marisa C. Bocklet, Adrianna R. Losquadro, Lynn E. Marsh, Ashleigh E. Outhous, Dr. Sam Morton and Dr. Chrisi A. Hughey | Curated Compound Library for Beer Processomics |
| Louis Bondurant, Olivia Swahn, Chunyi Guo and Dr. Daniel Downey | Lake Fertilization and Nutrient Budgets: Lake Management versus Chesapeake Bay Total Maximum Daily Load (TMDL) Reduction |

(Student presenters underlined)

| Oral Session II: Friday April 12, 2018 *(Festival Highlands)* | | |
|---|---|---|
| **1:30 pm** | Taylor L. Albertelli, Kendahl Ott, Heather Manring, Stuart Campbell, Maegen A. Ackermann and Dr. Nathan Wright | Towards the Inhibition of Calpain-Dependent Desmoplakin Cleavage in Arrhythmogenic Cardiomyopathies |
| **1:45 pm** | Spencer Grewe and Dr. Oleksandr Kokhan | Uncovering a Molecular Mechanism for Allosteric Regulation of the Cytochrome bc1 Complex |
| **2:00 pm** | Jacob A. Whitley, Aidan M. Ex-Willey, Daniel R. Marzolf, Maegen A. Ackermann, Anthony L. Tongen, Oleksandr Kokhan and Nathan T. Wright | Obscurin is a Semi-Flexible Molecule in Solution |
| **2:15 pm** | Isaac Miller, Ty Faulkner, John Saunier and Dr. Paul Raston | Laser Spectroscopy of OCS Dimers in 4He Nanodroplets |
| **2:30 pm** | Jackson White, Shaston Newman, Daniel Conway and Dr. Nathan T. Wright | A First Step Toward's Elucidating Obscurin's Molecular Mechanism |
| **2:45 pm** | Chris Angelelli, Kyle Wallenstrom, and Dr. Debra Mohler | Overcoming Degradation: A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs |
| **3:00 pm** | Isatu Kamara, James Harness and Dr.Tom Devore | Stripping water from air Using Magnesium sulfate Heptahydrate and Zinc sulfate Hexahydrate with Sunlight |

| Special Announcements *(ISAT 159)* | |
|---|---|
| **3:40pm** | Announcement of Chemistry and Biochemistry Student Award Winners |

| Keynote Address: Friday April 12, 2019 *(ISAT 159)* | | |
|---|---|---|
| **3:45 - 4:45 pm** | Lisa M. Christianson, MD, MPH<br>JMU Class of 1995 | Navigating the Sometimes Bumpy Road Through the Real World – Lessons for Approaching Life after Undergraduate School |

# Keynote Address

*Friday, April 12, 2019 at 3:45pm*
*ISAT Room 159*

## Navigating the Sometimes Bumpy Road Through the Real World – Lessons for Approaching Life after Undergraduate School

**Lisa M. Christianson, MD, MPH**
**(JMU Class of 1995)**
*University of Virginia Student Health Center*
*University of Virginia School of Medicine*
Charlottesville VA

Life after graduation can be easy for some, and more challenging for others. We are often led to believe that everyone else has a clear vision of what road they will travel, and exactly where they are going. Many of us are conditioned to believe we need to appear "put together" and that we need to constantly strive for "success", defined by our perception of the world's expectations. This recipe may work for many, and for others it may work, but come at an emotional or physical price. For still others it may not work at all, and this perception of failure to achieve certain milestones can lead to disappointment, and even be devastating for some. I present a somewhat brief, and hopefully a bit useful, summary of the path my life has taken, and what I have learned along the way, in hopes that it might help or inspire a few people out there who might not know exactly where they are going and how they are going to get there, or are struggling just to stay on the road.

# STUDENT ABSTRACTS

(Student presenters underlined)

**Purification and Characterization of the *E. Coli* Common Pilus Protein EcpD**

Benjamin W. Adams and Dr. Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Escherichia coli (E. coli) bacteria cause diarrhea through colonization of the digestive tract. To adhere and remain in the digestive tract, tiny hairs on the bacteria (fimbriae or pili) stick to both other bacteria and host epithelial cells. These pili are encoded by the ECP (*E. coli* Common Pilus) genetic cassette. Within this cassette, EcpA makes up the bulk of the pilus while EcpD comprises the tip, and is crucial for adhesion. While the structure and multimerization of EcpA is well known, virtually nothing is known about the structure EcpD. Here, we describe initial attempts to purify EcpD, in an effort to better structurally and characterize this protein. This work will eventually be used to better define immunogenic regions of EcpD, as well as elucidate the molecular mechanism of bacterial adhesion.

**Towards the Inhibition of Calpain-Dependent Desmoplakin Cleavage in Arrhythmogenic Cardiomyopathies**

Taylor L. Albertelli[1], Kendahl Ott[1], Heather Manring[2], Stuart Campbell[3], Maegen A. Ackermann[2] and Dr. Nathan T. Wright[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Physiology and Cell Biology, Ohio State University
[3]Department of Biomedical Engineering, Yale University

Desmoplakin (DSP) is a large (260 kD) protein found in the desmosome, a subcellular structure that links the cytoskeleton of one myocyte to that of its neighbor. In cardiomyocytes, desmoplakin's main function is to maintain cell-to-cell adhesion and synchronization during heart contractions. A mutation hot-spot, centered around the SH3 domain of DSP, is associated with arrhythmogenic cardiomyopathy, but the underlying mechanism(s) of this association isn't well studied. Here, we show that many of these disease-causing mutations display increased calpain sensitivity. Additionally, structural and computational studies on DSP variants show that this cleavage event is driven not through a gross structural change, but instead through the discrete exposure of a normally-occluded calpain cleavage site. Initial in silico and in vitro screens of small molecules suggest the feasibility of developing a pharmaceutical solution to prevent calpain-mediated DSP cleavage.

**Overcoming Degradation: A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs**

Chris Angelelli, Kyle Wallenstrom and Dr. Debra Mohler
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Antisense oligonucleotide analogs (ASOs) are therapeutic agents that consist of short or modified DNA or RNA molecules that bind to messenger RNA (mRNA) and prohibit the synthesis of a protein from transcribed mRNA. The potential of this technology is high and could prove to be an effective way to stop unwanted protein aggregations with specificity. ASOs face many challenges that include but are not limited to: membrane permeability, potency/concentration, non-specific effects, degradation by exonucleases, and shelf life. To combat these challenges, a novel synthetic strategy to form a 7-member carbon ring was performed. Thus far, Adenine, Uracil, and Thymine baes have been successfully attached to the synthetic 7-member carbon ring with low yields.

**Curated Compound Library for Beer Processomics**

Marisa C. Bocklet[1], Adrianna R. Losquadro[1], Lynn E. Marsh[1], Ashleigh E. Outhous[1], Dr. Sam Morton[2] and Dr. Chrisi A. Hughey[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Engineering, James Madison University

Dr. Hughey's research group has partnered with the Madison Academic Brewery (MAB) to study molecular changes that occur during the beer brewing process (a.k.a. beer processomics). In order to monitor these changes, we built a curated compound library from malt and hop compounds reported in the literature. Approximately 70 journal articles yielded a library of over 500 compounds. The Yeast Metabolome Database, which contains ~15k metabolites from brewer's yeast, will be used to monitor compounds produced and consumed during fermentation. These databases will be used to monitor molecular changes in a single hop, single malt (or SMaSH) beer produced by MAB in March. Samples were collected during the entire brewing processes. Currently, Dr. Hughey's research group and CHEM 352L are screening the final beer product with GC/MS and LC/MS to identify compounds present.

**Lake Fertilization and Nutrient Budgets: Lake Management versus Chesapeake Bay Total Maximum Daily Load (TMDL) Reduction**

Louis Bondurant, Olivia Swahn, Chunyi Guo and Dr. Daniel Downey
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Nitrogen and phosphorus entering the Chesapeake Bay must be reduced to meet the requirements of the Environmental Protection Agency (EPA) 2010 Chesapeake Bay Total Daily Maximum Load (TMDL). Lake fertilization by the Virginia Department of Game and Inland Fisheries (VDGIF) is long standing accepted management tool for fisheries enhancement to stimulate algal blooms. The intentional addition of fertilizers into recreational fishing lakes has been brought into question as contributing to nutrient loading of the Bay. To evaluate this concern, since March 2017 we have been conducting a comprehensive lake water chemistry evaluation of four lakes in the watershed of the Bay: Lake Brittle, Burke Lake, Huntsman Lake and Lake Shenandoah. The first two were fertilized by application of Sportmax® during the two summers included in the evaluation period. Samples were taken at each lake from feeder streams, tail waters and within-lakes, assayed and compared for the evaluation. More than twenty chemical and analytical parameters have been measured, with total phosphorus (TP) and total nitrogen (TN as $NO_3$-N + $NH_3$-N + organic N) of primary concern. Stream gauge data and rainfall records were used to develop loading and discharge values for water volume, that were combined with observed concentrations to give nutrient budget data. During the first season of sampling rainfall and runoff were slightly below average values. In the second year of the study, rainfall increased by more than 73%. Daily average nitrogen loads and discharge (kg/d) during the first year of the study were: Brittle (23, 17), Burke (44, 43), Huntsman (13, 28) and Shenandoah (56, 26). The first year daily average phosphorus loads and discharge (kg/d) were: Brittle (1.74, 0.57), Burke (5.38, 0.35), Huntsman (0.25, 1.07) and Shenandoah (0.41, 30). These data revealed that VDGIF lakes were storing nutrients, while the unfertilized Huntsman Lake was discharging nutrients, In year two, nitrogen loads and discharge (kg/d) were: Brittle (52, 34), Burke (23, 12), Huntsman (33, 32) and Shenandoah (77, 55), while the phosphorus values were Brittle (2.23, 1.24), Burke (5.85, 1.17), Huntsman 1.46, 1.95) and Shenandoah (0.38, 0.31). The values were greater in year two due to the high discharge, but nutrient nitrogen and phosphorus were again stored in VDGIF lakes and released from the unfertilized lake.

**Expression and Preliminary Characterization of GSU0105**

Tyler Brittain, Matt O'Malley and Dr. Oleksandr Kokhan
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

C-type cytochromes play an important role in the respiration of dissimilatory iron-reducing bacteria. They form extended conduits for charge transfer between the cellular metabolism and external electron acceptors such as particles of iron oxide, metal ions, and humic substances. However, very little is known about biophysical, biochemical, and structural properties of this large and diverse class of proteins. Out of more than 80 c-type cytochromes in Geobacter sulfurreducens, only about 10 have been previously characterized. Here we present our results on expression and preliminary characterization of GSU0105, a novel 3-heme cytochrome. We successfully cloned the gene and achieved acceptable expression in E. coli. A sufficient amount of protein has been isolated to perform UV-Vis, LC-MS, and SAXS characterization. The results of our preliminary characterization reveal that the protein has the expected mass and typical multiheme c-type cytochrome spectral properties. Despite a similar size (71 amino acids) and the same number of c-type hemes to the members of the cytochrome c7 family, multiple sequence alignment suggests the GSU0105 belongs to a new family of cytochromes. The protein is very prone to formation of long linear complexes likely caused by His-tags. Work is underway to create tag-free constructs in order to improve GSU0105 solubility, and therefore yield and enable crystallization trials.

**SAXS and MD studies on β-amylase 2 tetramer in Arabidopsis thaliana**

Nithesh P Chandrasekharan[1], Ian R. Roy[2], Dr. Jonathan D Monroe[3] and Dr. Christopher E Berndsen[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Health Sciences, James Madison University, Harrisonburg, VA 22807
[3]Department of Biology, James Madison University, Harrisonburg, VA 22807

Starch is an important component of the human diet as it is broken down into glucose to provide energy for metabolic reactions in the body. The amount and sources of starch that humans consume greatly varies around the world depending on the plants that are indigenous to each diet. In plants, starch is hydrolyzed into the disaccharide maltose by β-amylase enzymes, a process that is important night time metabolism and the response to stress in plants. By understanding starch regulation by β-amylases, we could potentially improve the quality of food crops which will benefit those who suffer from food insecurity and nutritional deficiencies.

Arabidopsis thaliana contains nine β-amylases (BAMs) that show distinct catalytic activities and functional regulation. Starch is located in the chloroplast and there are 4 chloroplastic BAMs. We are interested in understanding the functional and regulatory differences in these enzymes. The focus of our study is BAM2, which was recently found to be a tetramer and contain a secondary starch binding site which regulates BAM2 activity. Since there are no structures of BAMs from Arabidopsis, we aimed to characterize the structural mechanism of BAM2 regulation by starch binding to the secondary binding site. We first modeled BAM2 as a tetramer using previous experimental information and then performed simulations of this model in several substrate and starch bound states to understand the role of the secondary starch binding site on the active structure. We found that starch binding influences protein dynamics near the active site, which we suggest may be the basis for allosteric regulation. We further identified an amino acid which appears to regulate the T to R transition of the enzyme. We supported these computational studies with small angle X-ray scattering studies of BAM2 structure and with biochemical assays of amylase activity. These latter studies were aided by the development of a novel fluorescent biosensor assay of maltose production that allows for comparison of diverse substrates from small polysaccharides to soluble starch within a single continuous assay method. These comparisons indicate that BAM2 strongly prefers starch-like substrates over shorter polysaccharides, likely due to allosteric regulation by the secondary starch binding site. Current studies are focused on understanding the effects of this molecular mechanism on starch structure with the goal of elucidating the functional role of BAM2 in plants.

**The Effect of Varied TiO2 Coverages/Au (111) on Ethanol Selectivity**

Maria DePonte, David Boyle, Jeremy Wilke, Maxwell Z. Gillum, Hasan Kaleem, Daniel A. Schossler and Ashleigh E. Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Au (111) is an inert substrate that is transformed into an active model catalyst when modified with $TiO_2$ nanoparticles. The presence of $TiO_2$ acts as a source of oxygen on gold has shown to produce both the oxidative product, acetaldehyde, and the reduced product, ethylene, for ethanol (EtOH) reactions. In order to gain insight into the effect of $TiO_2$ coverage on Au (111) for selective ethanol chemistry, a systematic study investigating 1 minute, 1.5 minute, and 3 minute $TiO_2$ depositions was performed. Temperature programmed desorption (TPD) was used to study the high temperature desorption products after the adsorption of EtOH on the different $TiO_2$ coverages on Au (111). The morphology of the surface was studied using atomic force microscopy, and X-ray photoelectron spectroscopy was used to confirm the presence of TiO2 on Au (111). The selectivity in ethanol reactions over TiO2/Au (111) decreases as the coverage (and therefore nanoparticle size) of TiO2 increases: the percent formation of acetaldehyde 100%, ~70%-90%, and a max of ~70% for a 1 minute, a 1.5 minute, and a 3 minutes $TiO_2$ deposition, respectively. Oxidation of the model catalyst surface at elevated temperatures (600 K) promotes acetaldehyde formation, while oxidation at room temperature increases yield of all products.

**Study of the Lysine Deprotonation Mechanism in Ubiquitin Conjugating Enzyme, Ubc13**

Katherine Elliott[1], N. Cole Seward[1], Heath Hampton[2] and Dr. Isaiah Sumner[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807 ;
[2]Department of Biology, Gallaudet University

Ubiquitin (Ub) is a regulatory protein with the ability to flag proteins to be degraded by the proteosome. Ub is covalently attached to a lysine on the target protein by a series of reactions catalyzed by three types of enzymes: ubiquitin activating enzymes, E1; ubiquitin conjugating enzymes, E2; and ubiquitin ligases, E3. Before Ub is transferred to its target, it is bonded to the E2 via a thioester linkage. In this study, we examine the E2 enzyme, Ubc13, which catalyzes the formation of K63-linked polyubiquitin chains. The chains are formed when a lysine on the target Ub (K63) attacks the thioester bond between Ubc13 and the substrate Ub. To initiate this reaction, K63 on the target Ub must be deprotonated, turning it into an active nucleophile. There are two possible deprotonation sites: a conserved aspartate in Ubc13 (D119) and a conserved glutamate in the target ubiquitin (E64). In order to determine any preference between D119 and E64, we used classical molecular dynamics, Born-Oppenheimer molecular dynamics and single point QM/MM to model K64 deprotonation in several E2~Ub conjugates.

**Engineering a Cytochrome with a Tunable Bandgap Potential**

Samuel D. Fontaine[1], Coleman M. Swaim[1], P. Raj. Pokkuluri[2] and Dr.Oleksandr Kokhan[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807 ;
[2]Argonne National Laboratory, Lemont, IL 60439

We are exploring fundamental factors controlling electron flow in proteins and trying to apply these principles to create bio-hybrids that mimic properties of conventional semiconductors. To this end, we developed and extensively characterized 12 point mutations of PpcA, a 3-heme member of the cytochrome c7 family native to Geobacter sulfurreducens. These mutations were engineered to influence the redox potential (Em) of the middle heme (heme III) in PpcA by using four different strategies: performing charge reversal mutations, decreasing solvent access to the heme plane with bulky residues, altering the native bis-histidine axial ligation of the heme, and by attempting to form hydrogen bonds with the propionates of the heme. The latter strategy is expected not only to increase Em but also to introduce a redox Bohr effect. Out of 12 mutants, 11 were expressed in E.coli in sufficient quantities and show thermal stability in temperature-dependent CD experiments comparable to wild-type protein (Tm > 90Â°C). HPLC-ESI-MS was used to confirm both the purity and the mass of the expressed mutants. Small-angle X-ray scattering confirmed that the mutant proteins were folded correctly and formed the expected compact globular structures. Peroxidase activity assays were used to study flexibility and solvent exposure of heme binding pockets. Optical redox titrations have shown our ability to obtain reliable and reproducible data thereby allowing us to measure the effect of the mutations on the electrochemical properties of all 3 hemes and to understand the underlying principles and viable approaches in tuning relative heme redox potentials. Successful development of this project may lead to biological semiconductors with much smaller footprints and selectively tunable bandgap properties.

**Olefin Desorption Studies on Au (111)-Based Catalysts**

Maxwell Z. Gillum, Jeremy A. Wilke, Maria C. DePonte, Eric M. Maxwell, Daniel S. Schlosser and Dr. Ashleigh E. Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

The partial oxidation of olefins, such as ethylene and propylene, creates industrially important products that are used in a multitude of chemical fields ranging from food processing to polymer production to automotive chemistry. Olefin research is being conducted using metal/oxide model catalysts, as they have shown an affinity for high selectivity oxidation reactions. However, the fundamental interactions of olefins on these surfaces are not yet well understood. To gain a comprehensive understanding of olefin intermolecular and surface interactions, temperature programmed desorption (TPD) studies were conducted using Au (111) based model catalysts with different surface preparations. Desorption kinetics of ethylene and propylene were studied on pristine, oxygen covered, and titania modified Au(111) surfaces. Desorption products were monitored using quadrupole mass spectrometry and the surface morphology was analyzed using ex-situ atomic force microscopy (AFM). The presence of titania was confirmed via X-ray photoelectron spectroscopy (XPS). By understanding the characteristic behaviors with combined experimental techniques, a more comprehensive understanding of the surface interactions between small alkenes and Au based catalysts may be identified.

**Uncovering a Molecular Mechanism for Allosteric Regulation of the Cytochrome bc1 Complex**

Spencer B. Grewe and Dr. Oleksandr Kokhan
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

The cytochrome bc1 complex (Complex III, ubiquinol-cytochrome c oxidoreductase) is a highly conserved multi-subunit protein found in the mitochondria and is a key complex in the electron transport chain. During oxidative phosphorylation, cytochrome (cyt) c, a mobile electron carrier, binds to one cyt c1 subunit of a bc1 complex dimer and shuttles electrons from Complex III to Complex IV. X-ray crystallographic studies revealed that only one molecule of cyt c binds to one bc1 complex dimer, despite two cytochrome c1 subunits available for binding, pointing toward the existence of a regulation mechanism preventing the docking of a second cyt c substrate. However, a structural basis for such a mechanism of long-range (>30Å) regulation of substrate binding beyond the typical range of electrostatic repulsion is not clear from static structural studies alone. We employed all-atom molecular dynamics simulations to uncover a possible mechanism of regulation. Our results reveal that a finger-like extended domain of the vacant cyt c1 subunit undergoes a conformational change with its tip moving towards cyt c, transferring mechanical motion and causing distortion of the vacant cyt c1 binding site. A change in the local lipid content of the membrane from polar POPC to charged cardiolipin interrupts this effect, implying the regulation of this mechanism by local membrane potential. In addition, we explored the role of naturally occurring methylated Lys-72 residue of cyt c in substrate binding and its potential role in the regulation of activity of the bc1 complex.

**Pitt Springs Run: A Tale of Two Water Chemistries**

Chunyi Guo, Erika Hutchinson and Dr. Daniel M. Downey
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Devonium Group post-Tonoloway limestone, Needmore Formation and Millboro (Martinsburg) Shales which are soluble rocks that provides plenty of carbonate. In 2010, the US Forest Service began an experimental limestone treatment strategy to enable trout survival upstream of the spring. There has been limited success due to access limitations and other issues since that time. The results of water chemistry monitoring by JMU for this cooperative project from 2010-2018 will be presented in this poster. Problems that have occurred and recommendations will be discussed in the context of how water chemistry values tie to practicalities of management in the field.

**LAKE KEOKEE: Physical -- Chemical Parameters, Fish Populations and Management Issues**

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

The Virginia Department of Game and Inland Fisheries Keokee Dam impounds a 98 acre reservoir near the headwaters of the North Fork Powell River Lee County, Virginia. Lake Keokee's purpose is to provide public recreational fishing in a rural mountain setting. Fish recruitment and growth have not met the expectations of fisheries managers and anglers. Lake Keokee has been treated with limestone to control iron floc and fertilized with a nitrogen-potassium-phosphorous mix. The goals of this project were to analyze Lake Keokee water chemistry and sediments, watershed characteristics, geology and lake morphology to provide data for fisheries managers. Inductively coupled plasma-mass spectrometry was used to measure trace elements: iron, aluminum, magnesium and arsenic. Major ions were determined by ion chromatography. Total phosphorous and chlorophyll a were measured colorimetrically and by fluorimetry, respectively. Total phosphorous, chlorophyll a and Secchi disk measurements were used to calculate the Trophic State Index (TSI). Sediment samples were taken at multiple locations in the lake and dam and analyzed for iron, aluminum, magnesium, zinc and lead. The results of the analyses and fish surveys from 2012 to 2018 will be presented along with recommendations for lake management.

**Investigation of the Ammine-Copper-Oxalate System**

Tabitha J. Hain, Dr. Barbara A. Reisner and Dr. Thomas C. DeVore
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Research on the phases of the ammine-copper-oxalate system has been done sporadically for over a century. Three phases of $(NH_3)_2CuC_2O_4$ (α, β, γ), $NH_3CuC_2O_4$, and $(NH_3)_2CuC_2O_4 \cdot 2H_2O$ have been reported in the literature, but the true number of phases of $(NH_3)_2CuC_2O_4$, their structures, and the transformations between them remain unclear. Attempts were made to reproduce the syntheses of these compounds to investigate their potential as heat storage materials, resulting in relatively pure $(NH_3)_2CuC_2O_4 \cdot 2H_2O$, γ-$(NH_3)_2CuC_2O_4$, and $NH_3CuC_2O_4$. Although it was found that they are not good candidates for heat storage, their structures and decompositions were studied using PXRD, TGA, and DSC. Variable temperature PXRD is being used to elucidate structural transformations between the phases. Our current understanding of this system will be presented.

**Synthesis and Characterization of Palladium(II) Complexes with Substituted N-Pyrazolylpropanamide and N-Trizaolylpropanamide Derivatives**

Sara Hildebrand, Dr. Donna S. Amenta and Dr. John W. Gilje
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Four derivatives have been synthesized through base catalyzed Michael additions, with Triton B as the basic catalyst. Reaction of methacrylamide and 1H-1,2,3-triazole produced 1, an asymmetrically substituted triazole with a methylpropanamide moiety. The reaction of N-isopropylacrylamide and 1H-1,2,3-triazole produced two isomeric substituted triazoles, one with the N-isopropylpropanamide substituent bonded to the exterior ring nitrogen (2), the other with the substituent bonded to the central nitrogen (3). The reaction of diacetone acrylamide with pyrazole produced 4, an asymmetrically substituted pyrazole. All compounds have been characterized through NMR and IR spectroscopy as well as elemental analysis. Additionally, compounds 1 and 4 have been characterized through single crystal X-Ray diffraction. Derivative 1 was reacted with dichloro(1,5-cyclooctadiene)palladium(II) and the product was characterized through IR spectroscopy. No reaction occurred when derivatives 2 and 3 were reacted with dichloro(1,5-cyclooctadiene)palladium(II). The reaction of dichloro(1,5-cyclooctadiene)palladium(II) with 4 displaces cyclooctadiene, forming complex 5. The complex has been characterized through NMR and IR spectroscopy, elemental analysis, and X-Ray diffraction. The chemistry of these derivatives with other transition metal complexes is currently being investigated.

**Stripping water from air Using Magnesium sulfate Heptahydrate and Zinc sulfate Hexahydrate with Sunlight**

Isatu Kamara, James Harness and Dr. Thomas C. Devore
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The reversible reactions of hydration and dehydration of anhydrous salts has been suggested as a possible way to harvest liquid water from the air using sunlight as a primary heat source. Salt hydrates such as magnesium, zinc, and copper sulfates as well as copper chloride have been shown to be the most promising materials for this purpose. These compounds were prepared by dissolving the commercial stock salts in demonized water and then allowing the excess water to evaporate in order to obtain the required salt hydrate crystals or were used ass received. The thermal hydration/dehydration of these compounds were investigated using FT-IR, TGA, DSC, and variable temperature on powder X-Ray diffraction. Observation from PXRD the dehydration process as the materials were heated, $ZnSO_4$ was observed the starting material to be a mix of 6 and 7 water dehydrate to uncharacterized intermediates and amorphous phases before the final dehydrated monohydrate product which was observed in a vacuum of TTK at 25˚C for 4 hours 20 mins per hour scanned. The DSC was used to determine the enthalpies of formation for zinc sulfate Hexahydrate is 238.8KJ/mol of dehydration and magnesium sulfate heptahydrate. From TGA, the initial water loss is 34.149% for 3 moles of $H_2O$ with a total mass loss of 41.388%. for $ZnSO_4.7H_2O$, and $MgSO_4.7H_2O$ shows three steps mass lost.

**Kinetic Studies of 2-(2'-hydroxyphenyl) benzenesulfinate desulfinase substrate analogs**

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2-(2'-hydroxyphenyl) benzenesulfinate desulfinase (DszB) is an enzyme that catalyzes the cleavage of the carbon-sulfur bond as the final step of the desulfurization of 2-(2'-hydroxyphenyl) benzenesulfinate (HPBS) producing sulfite and 2-hydroxybiphenyl (HBP). This reaction is used to study the biodesulfurization of dibenzothiophene, the major organosulfur compound found in fossil fuels/petroleum. Previous studies in the Watkins lab suggested that halogenated analogs of HPBS are competitive inhibitors of DszB, so a coupled assay was used to test their effect on kinetic activity. The relative activity of these analogs was tested measure both products of the reaction. The rate of HBP formation was monitored using a fluorometric assay with an excitation at 288 nm and measuring emission at 414 nm. The rate of sulfite product formation was measured in the coupled assay with Sulfite Oxidase (SOX) by analyzing a change in absorbance at 540 nm. When testing the analogs HPBS-Cl and HPBS-Br for activity, no product was detected. When measuring enzyme activity in the presence of the halogenated analogs and the substrate HPBS, an increase in DszB activity was observed, with HPBS-Cl and HPBS-Br showing an increase product formation of 475% and 213%, respectively. Individually these HPBS analogs did not act as catalytic substrates or competitive inhibitors, however when coupled with HPBS the analogs acted as activators. Based on these results, we are exploring the structure of DszB to further understand how HPBS analogs can affect the desulfinase kinetics.

**The Structure and Functional Characterization of the *Leishmania donovani*'s Ufm-ylation Pathway**

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Ubiquitin fold modifier 1 (Ufm1) an ubiquitin-like protein and Ubiquitin fold modifier activating enzyme (Uba5, E1) are proteins found in eukaryotic organisms that play a crucial role in cell cycle regulation, signal transduction, and ER stress. Leishmania donovani (Ld) is a trypanosomatid parasite that has been shown to have enzymes homologous to Uba5 and Ufm1. Leishmania Ufm1 and Uba5, as well as the substrate-targeted proteins, are associated with the mitochondria which have not been observed in other organisms. This suggests that these Leishmania proteins may have physiological roles not yet described in other organisms. Leishmania donovani causes leishmaniasis, a disease that is accompanied by sores and lesions that will appear at varying depths of the body depending on the type and increases the host's susceptibility to co-infection with other diseases. There are currently no effective vaccines for leishmaniasis. LdUfm1, an N-terminally truncated form of LdUfm1, and LdUba5. LdUfm1 and LdUfm1(tr.) were successfully purified and were characterized with SEC-MALS. We then performed gel migration shift assays to demonstrate the compatibility of the human and Leishmania systems to conjugate LdUfm1. We found that full-length Leishmania Ufm1 but not the truncated form were viable substrates for human Uba5, suggesting a role for the N-terminus of Ufm1 conjugation. We are currently working to purify LdUba5 further for functional and structural comparisons to the human enzyme. Additionally, we began setting crystal trays to obtain protein crystals for structure determination. We have preliminarily obtained crystals of the truncated Ufm1. Future work will optimize these crystals, perform further experiments for structural characterization and explore the cross-reaction between the human and Leishmania enzymes. Characterization of the Leishmania donovani conjugation pathway could facilitate the development of therapeutic treatments for leishmaniasis.

**Synthesis and Antibacterial Study of Tetracationic Amphiphiles**

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Significantly high rates of illness and death caused by antibiotic resistant bacteria is an increasing concern in healthcare, specifically in hospital settings. According to the Center for Disease Control and Prevention, a high volume of patients has been infected with healthcare-associated infections while hospitalized. One approach to addressing this issue, is the synthesis and study of novel antiseptics. To this, end, a series of bis-bipyridinium tetracationic amphiphiles were synthesized with varying tail lengths ($C_6H_{13}$ – $C_{12}H_{25}$) and linker lengths ($C_5H_{10}$ – $C_{16}H_{32}$). Minimum inhibitory concentration (MIC) values were determined against several strains of bacteria for each of the molecules in this study in order to better understand the relationship between surfactant structure and antibacterial activity. Analysis of data collected thus far suggests that amphiphiles in this series with short tails and long linkers demonstrate the highest antimicrobial potency. Ongoing work will focus on fully characterizing this new series of amphiphiles and collecting and analyzing MIC values for recently synthesized derivatives.

**Laser Spectroscopy of OCS Dimers in $^4$He Nanodroplets**

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Quantum-cascade laser spectroscopy was used to characterize OCS dimers embedded in $^4$He nanodroplets. Rovibrational bands corresponding to the polar parallel and nonpolar "sulfur-in" dimers, which have previously been characterized in the gas phase, were detected in addition to a third dimer which has been predicted by theory but heretofore undiscovered experimentally. This dimer has a nonpolar, "oxygen-in" configuration and was characterized in part using Stark spectroscopy.

**Towards the inhibition of calpain-dependent desmoplakin cleavage in arrhythmogenic cardiomyopathies**

Kendahl L. Ott[1], Heather Manring[2], Stuart Campbell[3], Maegen Ackermann[2] and Dr. Nathan T. Wright[1]
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[2]Department of Physiology and Cell Biology, Ohio State University;
[3]Department of Biomedical Engineering, Yale University

Desmoplakin (DSP) is a large (260 kD) protein found in the desmosome, a subcellular structure that links the cytoskeleton of one myocyte to that of its neighbor. In cardiomyocytes, desmoplakin's main function is to maintain cell-to-cell adhesion and synchronization during heart contractions. A mutation hot-spot, centered around the SH3 domain of DSP, is associated with arrhythmogenic cardiomyopathy, but the underlying mechanism(s) of this association isn't well studied. Here, we show that many of these disease-causing mutations display increased calpain sensitivity. Additionally, structural and computational studies on DSP variants show that this cleavage event is driven not through a gross structural change, but instead through the discrete exposure of a normally-occluded calpain cleavage site. Initial in silico and in vitro screens of small molecules suggest the feasibility of developing a pharmaceutical solution to prevent calpain-mediated DSP cleavage.

**Using COPUS to Inform Teaching in Foundation Inorganic Chemistry Courses**

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The goal of the VIPEr fellows project is to help faculty reflect on their teaching, redesign their foundation inorganic chemistry course to incorporate active learning strategies, and understand the effects of the community on faculty practice and student learning. This portion of the project focuses on analyzing classes using the Classroom Observation Protocol for Undergraduate STEM (COPUS) to see what instructors and students do during the class. Videos of inorganic courses from VIPEr fellows were processed and coded. To code these classes, the COPUS codes were refined to fit activities that happen in inorganic chemistry classes. Once coded, inter-rater reliability was verified with the Cohen's kappa statistic, and discrepant events were discussed and used to modify the coding. This data will be used to allow instructors to reflect on their practice and identify changes they would like to make in their instruction.

**Partial Molar Volumes and Volume of Mixing of Salts and Osmolytes**

Masha Pozhilenko, Will Vakay and Dr. Yanjie Zhang
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This is a study of solute-solvent interactions through volumetric analysis. Densities of anion and cation salts from the Hofmeister series and seven osmolytes at varied concentrations were measured to determine the apparent molar volume of the solute, partial molar volume of solvent and solute, and volume of mixing in aqueous solutions. In general, strongly hydrated salts showed smaller limiting partial molar volume compared to weakly hydrated salts. Volume of mixing values were more negative for strongly hydrated anions and cations suggesting that the interactions of these salts with water were more favorable. Based on these trends the osmolytes can be assessed. Detailed volumetric analysis of solute-water system will be presented.

**Surface Characterization of Ethanol Desorption from Silver (111) Defective Sites**

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Silver (Ag) is an ideal model catalyst for ultrahigh vacuum science due to its simple catalytic mechanism for carbon monoxide oxidation as well as its possible uses in catalytic converters, and photo- and electro- catalysts. Ethanol can be used as a fuel in vehicles and through the ethanol oxidation reaction, the latter of which is catalyzed by palladium/silver nanoparticles. The goal of the research herein is to better understand the interaction of ethanol molecules on defective sites of Ag (111) to mimic active sites found on Ag nanoparticle catalysts. The interaction between ethanol (EtOH) and Ag (111) the most stable facet of silver and most commonly exposed facet for fcc nanoparticles - was studied using temperature programmed desorption (TPD) and X-ray photoelectron spectroscopy (XPS), and the morphology of the Ag(111) surface was studied using atomic force microscopy (AFM). The presence of defective sites alters the adsorption and desorption of EtOH from Ag (111) and has implications for photo- and electro- chemistry catalysis. A better understanding of defect dependent behavior for ethanol on silver can lead to a greater insight in to high surface area nanoparticle catalysts used in industry, catalytic converters, and electrocatalysis.

**Two synthetic approaches in the formation of a guanosine analog: connecting 2-amino-6-chloropurine to a novel 7-membered cyclic alkene alcohol**

Nicholas J. Valle and Dr. Debra Mohler
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Antisense oligonucleotide drugs act during translation by annealing to a faulty mRNA transcript, resulting in the degradation of the drug-mRNA complex. This therapy has had recent success in treating multiple sclerosis, and several studies have examined its capability to treat other neurodegenerative diseases. Our group aims to create antisense oligonucleotides containing carbon only backbones, rather than sulferdiester or phosphodiester backbones, in hopes of improving drug viability in the cell. In the first approach the novel cyclic alkene, a guanine precursor (2-amino-6-chloropurine), triphenylphosphine and diethyl azodicarboxylate (DEAD) were added to THF to facilitate the addition of the purine precursor to the alkene via a well-studied mechanism known as the Mitsunobu Mechanism. Column chromatography was utilized in an attempt to separate the desired product form the reaction mixture. A second approach attempted to add the purine precursor to the alkene via a simple substitution reaction model. The alkene was first prepared as an electrophile by substituting the alcohol with a mesolate group. In the substitution reaction, the nitrogen number 9 was deprotonated using sodium hydride, and the novel alkene with mesolate attached was added into the mixture. Proton NMR was used to identify products in both approaches. NMR data suggest the first approach was successful in creating the desired product, but the second approach was not. However, these data also suggest the formation of a triphenylphosphine-DEAD adduct, making the separation of the desired product from the reaction mixture exceedingly challenging. In the second approach, it is suspected that solubility differences between the purine nucleophile and the novel alkene electrophile lead to the reaction's failure. A new method for separation in the first approach and a solution for solubility differences in the second will be needed if they are to be considered effective at producing the desired nucleoside analog.

**A First Step Toward's Elucidating Obscurin's Molecular Mechanism**

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Obscurin is a giant (800-950 kDa) cytoskeletal protein involved in mobility and adhesion signaling pathways. It is the second most mutated gene in breast and colorectal cancers, and in muscles mutated obscurin leads to muscular dystrophy and cardiomyopathy. Obscurin's specific role in these diseases remains an active area of research. In an effort to better understand obscurin's molecular mechanism of action, here we describe an experimental approach to elucidate obscurin binding partners in eukaryotic cells. We have designed a series of constructs containing a promiscuous biotin ligase, and transfected this DNA into MDCK II epithelial cells. The resulting microscopy images, SDS-PAGE gels, and MS/MS data give us our first understanding of obscurin subcellular localization in non-muscle cells and provide a proof-of-concept platform to conduct future BioID assays on similar samples to identify specific binding partners.

**Obscurin Is a Semi-Flexible Molecule in Solution**

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Obscurin, a giant modular cytoskeletal protein, is comprised mostly of tandem immunoglobulin-like (Ig-like) domains. This architecture allows obscurin to connect distal targets within the cell. The linkers connecting the Ig domains are usually short (3-4 residues). The physical effect arising from these short linkers is not known; such linkers may lead to a stiff elongated molecule or, conversely, may lead to a more compact and dynamic structure. In an effort to better understand how linkers affect obscurin flexibility, and to better understand the physical underpinnings of this flexibility, here we study the structure and dynamics of four representative sets of dual obscurin Ig domains using experimental and computational techniques. We find in all cases tested, tandem obscurin Ig domains interact at the poles of each domain and tend to stay relatively extended in solution. NMR, SAXS and MD simulations reveal that while tandem domains are elongated, they also bend and flex significantly. By applying this behavior to a simplified model, it becomes apparent obscurin can link targets more than 200 nm away. However, as targets get further apart, obscurin begins acting as a spring, and requires progressively more energy to further elongate.

**Colloidal and Antibacterial Studies of Novel Polycationic Amphiphilic Polymers**

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A significant challenge facing the medical field is the proliferation of bacteria that are resistant to modern antibiotics (e.g., Methicillin-resistant Staphylococcus aureus, or MRSA). New antibacterial compounds are therefore important targets for medical applications, and industrial and agricultural cleaning procedures. We have synthesized three new amphiphilic cationic polymers, referred to as (M-12)12, (M-18)12, and (M-22)12, which possess the potential for antibacterial activity. Microwave heating was utilized in synthesizing these novel polymers, which were subsequently washed with solvent and dried *in vacuo*. Nuclear Magnetic Resonance (NMR) and Atomic Force Microscopy (AFM) were utilized to investigate structure and morphology of these cationic polymers. NMR spectra are consistent with the target polymer structures. AFM experiments suggest that (M-12)12 is capable of forming both micelles and vesicles in water. Preliminary biological studies demonstrate that the polymers impair bacterial growth. Ongoing work includes the preparation of additional derivatives, as well as additional biological and colloidal examination of these polymers.

**Investigation of donor/accepter properties of a fluorene based small molecule for flexible solar cell applications**

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

Our lab has previously developed an inorganic cluster $Co_6Se_8(Br(C_4H_2S)P(Ph)_2)_6$ (**1**), which has shown promising results as an acceptor as well as reduced phase separation with poly-3-hexylthiophene (P3HT). Interestingly the HOMO/LUMO levels and broad absorption range of **1** suggest that it may also be an effective acceptor material. The investigation of the donor/accepter versatility of **1** was performed with a small molecule acceptor. A new small molecule acceptor was synthesized in two steps in good yields. A synthetic intermediate, 2,7-Bis(5-formyl-2-thienyl)-9,9-dioctyl-9H-fluorene **(2)**, was made using 2,2'-(9,9-Dioctyl-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) **(3)** and 3-bromo-2-thiophenecarbaldehyde **(4)** under Suzuki conditions. Malononitrile **(5)** was added to the compound **(1)** to obtain a final product, 7,7'-(9,9-dioctyl-9H-fluorene-2,7-diyl) 5-[2-(2-thienyl methylene) malononitrile **(6) (FTM)**. Structural characterization of the material was done with $^1$HNMR, $^{13}$CNMR, FT-IR and PXRD. Optical and electronic characterization was done using cyclic voltammetry, UV-vis and fluorescence spectroscopy.

A series of fluorescence quenching experiments were performed to observe donor/acceptor interactions of $P_3$HT:FTM, and a control mixture of $P_3$HT:PCBM. To complement the solution state measurements, the solid-state morphologies of the systems were studied using atomic force microscopy. Devices were fabricated on ITO treated glass by spin casting 1:1 $P_3$HT:FTM or 1:1 $P_3$HT:PCBM from chlorobenzene, aluminum top contacts were then deposited using e-beam evaporation. Control devices ($P_3$HT:PCBM) displayed $I_{sc}$ =-0.00013 mA, $V_{oc}$=0.34 eV, and FF=17%, while $P_3$HT:FTM devices displayed $I_{sc}$ =-0.00034 mA, $V_{oc}$=0.31eV, and FF=24%. These results indicate that FTM has the potential to be an effective and easily modifiable acceptor material. Preliminary experiments indicated minor acceptor/donor interactions for the **1**: FTM system however additional experiments need to be performed to fully understand these interactions.

**Design a Synthesis of Dipeptide-Boronic Acid Gelators**

Avery York, Kevin Dannaher and Dr. Gretchen Marie Peters
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Supramolecular gels derived from biomolecules are of great interest due to their potential as biocompatible and biodegradable materials for sensing and targeted drug delivery applications. In particular, supramolecular gels derived from dipeptides are known to be suitable for a number of biomedical applications, including tissue engineering. While the gelating potential of dipeptides has been established, there remains an interest in developing new gelating systems and novel ways to incorporate pertinent targets into the gel network. The goal of our project was to synthesize a dipeptide gelator with a boronic acid handle that can be used to bind to different diol-containing biomolecules and drugs. We successfully synthesized a boronic acid dipeptide in three steps with 88% yield and fully characterized the product by $^1$H NMR. This dipeptide gels In future, we will continue to study the physical properties of this material as well the boronic acid dipeptide's ability to bind to diol-containing drugs.

## 2019 Department of Chemistry and Biochemistry Student Award Winners

| | |
|---|---|
| Amenta Award | Sara Hildebrand |
| R.D. Cool Award | Erin Krist |
| J.W. Chappell Scholarship | Matthew Hershberger |
| Palocsay Award in Undergraduate Research | Jackson White |
| Service Award | Adrienne Lee |
| J. W. Chappell Award | Melissa Hart |
| American Institute of Chemists | Nithesh Chandrasekharan |
| Degesch America Award | Amy Fox |
| ACS-Award | Rebekah Soliday |
| Casali Scholarship (May, 2018) | Amy Fox |
| CRC First Year Student Award (Spring, 2018) | Eric Maxwell |
| CRC First Year Student Award (Spring, 2019) | Olivia Mumma |
| Outstanding Student Researcher Award | *to be announced* |

Divisional Awards

| | |
|---|---|
| Biochemistry Award | Jake Whitley |
| ACS Analytical Award | Spencer Grewe |
| ACS Environmental Award | Louis Bondurant |
| ACS Inorganic Award | Tabitha Hain |
| ACS Organic Award | Tyler Miller |
| ACS POLYED Organic Award | Skyler Clark |
| ACS Physical Award | Isaac Miller |

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