

**WILLIAM PATERSON UNIVERSITY  
OF NEW JERSEY  
COLLEGE OF SCIENCE AND HEALTH**

# RESEARCH



**INTERNSHIPS AND EXTERNSHIPS  
GARDEN STATE — LOUIS STOKES ALLIANCE FOR  
MINORITY PARTICIPATION**

**GS-LSAMP**



**CELEBRATING STUDENT RESEARCH ACTIVITIES 2020  
ELEVENTH EDITION**

**EDITED BY: DR. DANIELLE DESROCHES, COVER BY RITA LEVINE**

***RESEARCH  
INTERNSHIPS, EXTERNSHIPS***

**WILLIAM PATERSON UNIVERSITY**

**COLLEGE OF SCIENCE AND HEALTH  
BIOLOGY DEPARTMENT**

**Garden State-Louis Stokes Alliance for Minority Participation (GS-  
LSAMP)**

**&**

**Minority Association of Pre-medical Students (MAPS)**

***Celebrating Student Research Activities***

***2020***

**11<sup>th</sup> Annual Edition**

# TABLE OF CONTENTS

## Introduction

*Dr. Danielle Desroches*

## Research Internships

William Paterson University, Biology Department

**Detecting Differences between Honeybee Gut Microbiomes in a Rapid SYBR qPCR Assay.**

*Jennifer Louis, Jake Bejarano, Dr. Martin (Mentor), Dr. Gilley (Collaborator).*

**Characterization of New Cryptochromes in the Dinoflagellate *Karenia brevis*.**

*Alan Abboud, Dr. Emily A. Monroe (Mentor).*

**Testing the Transcriptional Disruption Resulting from Integration of Two Reporter Constructs at the MPP10-YJR003C Genomic Locus on Chromosome XII in Budding Yeast.**

*Sarah Elkamhawy, James Arnone, PhD (Mentor).*

**Mechanism of Tail Resorption in Anuran Tadpoles.**

*Ma. Veronica Holganza, Jaishri Menon (Mentor).*

**An inexpensive operant chamber that collects cognitive data 24/7.**

*Jamie Carolyn Reulbach, David Freestone, and Dr. Bierbower (Mentor).*

**Determination of echinocandin antifungal susceptibilities following ectopic expression of medically relevant *FKSI* mutations in *Candida glabrata***

*Indira Sawh, Dr. K. Healey (Mentor).*

**Spider and Insect collection into taxonomy and information gathering**

*Marco Ortega, Dr. J. Spagna (Mentor).*

**Characterization of Gene Expression Pattern Changes in *Saccharomyces cerevisiae* as a Function of Genomic Distribution.**

*Khizar Siddiqui, Reem Eldabagh, Dr. Jonathan J. Foley, IV, Dr. James T. Arnone (Mentor).*

## William Paterson University, Chemistry Department

***De Novo* Approach Towards the Asymmetric Synthesis of Purposamine.**  
Terrence Hopkins, Dr. George A. O'Doherty (Mentor).

**Non-precious metal catalyzed direct synthesis of Guerbet alcohol.**  
Emir Sehovic, Parminder Kaur (Mentor).

Functionalization of C sp<sup>3</sup>-H Bonds via Copper Catalyzed Electrochemistry.  
Leslie Trigoura, Dr. Yalan Xing (Mentor).

**Ni/Cu-catalyzed oxidative C-H functionalization: Direct synthesis of allylic esters.**  
Jonathan McTague, Cassidy Anderson, and Dr. Parminder Kaur (Mentor).

**Patterns in Protein Flexibility.**  
Chris Reinknecht, Dr. David A. Snyder (Mentor).

**Accelerating the discovery of multilayer nanostructures with analytic differentiation of the transfer matrix equations.**  
James F. Varner, Dayanara Wert, Aya Matari, Raghad Nofal, and Jonathan J. Foley.

**Multi-Step Synthesis of the Natural Product Actinopolymorphol B.**  
Adriana Brandes, Maria Holganza, Alex Hildalgo, Claudia Kim, Chiara St Amant, Dr. Yalan Xing PhD (Mentor).

**Optimizing the anti-reflective solar cell coatings by using the differentiation of the transfer matrix equations.**  
Aya Matari, Dr. Jonathan Foley (Mentor).

**Synthesis of magnetic Iron Nanoparticles gels of *n*-(2-aminoethyl)-3-aminosilanetriol.**  
Zoraya Perez, Qiaxian Johnson, Dr. Bhanu P. S. Chauhan (Mentor).

## William Paterson University, Environmental Sciences Department

**Extinction of Iconic Megatoothed Shark Otodus megalodon: Preliminary Evidence from 'Clumped' Isotope Thermometry.**  
Chelesia Clarke, Allison Neumann, Shana Foster, Drew Pedersen, Troy Nixon, Clint Mautz, Dr. Michael Griffiths, Dr. Martin Becker, William Paterson University; Dr. Kenshu Shimada, DePaul University; Dr. Sora Kim, University of California Merced; Dr. Robert Eagle, University of California Los Angeles; Harry Maisch IV, The City University of New York.

***Enchodus* from the Arkadelphia Formation-Midway Group Contact (K-Pg), Hot Spring County, Malvern, Arkansas: Implications for the effects of the K-Pg Mass Extinction Event on a Piscivorous Food Web.**  
Michaela Gardener, Dr. M. Becker (Mentor).

**Meeting /Presentations**  
**Conferences Photographs**  
**Student awards**

**GS – LSAMP 10<sup>th</sup> Annual Conference**

**Rutgers: 10<sup>th</sup> Annual Conference – October 11, 2019**



**GS – LSAMP 10<sup>th</sup> Annual Conference**  
**Rutgers: 10<sup>th</sup> Annual Conference – October 11, 2019**



# Introduction

This is the 11th year the Garden State Louis Stokes Alliance for Minority Participation (GS-LSAMP) program has put together such publication in order to recognize the research efforts and successes by William Paterson University science majors.

As in previous years, Summer Research Internships and Externships have provided students with the opportunity to work on or off campus, in a laboratory or in their field of interest, under the supervision of a faculty. Such opportunity has allowed them to experience firsthand “how scientists work” and how to conduct scientific research. Many actively participated in specific projects, learn new techniques including the use of elaborate laboratory equipment, computer -assisted analyses, animal husbandry and handling, to name a few. Others have spent their summers volunteering or shadowing physicians in Hospitals and Health Clinics. Such internship has proven to be a valuable asset for students applying to Graduate or Professional school, or in job placement or career selection following graduation.

All the summer interns have presented their summer experience at one of our monthly, well attended, meetings in the Fall 2019 and Spring 2020 ( on campus and virtually) semesters. Additionally, several GS-LSAMP students had been planning to present their work at the Undergraduate Research Symposium which would have taken place at WPU in April 2020 now postponed due to the pandemic, . Others have gone to Regional meetings, including GS-LSAMP Annual STEM meeting at Rutgers University (October 2019). Five of our students won first Place . Most of these abstracts or summaries are in their own words and represent an honest and candid account of their work. Other abstracts are more formal and were presented at a national scientific meeting. Several of the projects were published in Peer Reviewed journals. These summer internships would not have been possible without the support of the Biology, Chemistry and Environmental Sciences faculty who have volunteered to mentor our students. Others have provided contacts for off campus opportunities.

This past summer, GS-LSAMP was able to provide stipends to 15 students. This support as well as this publication would not be possible without the support of Dr. Venkat Sharma , Dean of COSH who funded 10 more students, and of Dr. Jean Fuller-Stanley, Associate Dean of CSH, LSAMP project director at WPU. Many thanks to the previous Provost, Dr. Sandra DeYoung for providing the additional funding needed, Thanks to his support, an additional 8 students were funded. In addition, Dr. Donna Rennar -Potacco , Director of the SEC provided support for 4 of the applicants . **A total of 42 students** were involved, our largest group since the start of the GS-LSAMP program. A big thank you as well to Rita Levine for assisting in all matters related to GS-LSAMP and for her technical and graphic support with this manuscript.

We hope that next’s year publication will include many more interns and mentors.

## ***Dr. Danielle Desroches***

Professor

Human Physiology and Neuro-endocrinology, PhD

Integrated Math and Sciences (IMS) Director

Anatomy and Physiology Coordinator

Minority Association of Pre Medical Students ( MAPS) Coordinator

Biology Biotechnology Club ( BBC) Faculty Co Advisor

Garden State Louis Stokes Alliance for Minority in Sciences, ( GS-LSAMP) Academic Coordinator

[desrochesd@wpunj.edu](mailto:desrochesd@wpunj.edu) (973) 720-2329

# GS-LSAMP STUDENTS FUNDED : SUMMER 2019 - RESEARCH TOPICS

Name

Mentor

Department

## Research Internships Abstracts

### William Paterson University, Biology Department

Detecting Differences between Honeybee Gut Microbiomes in a Rapid SYBR qPCR Assay.

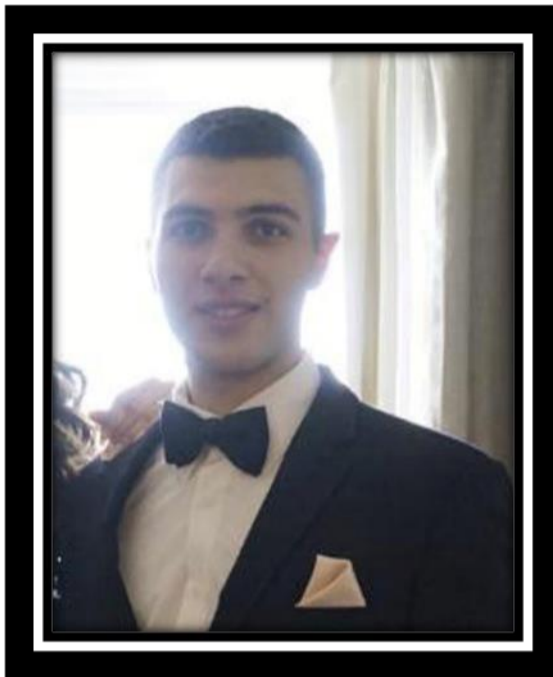


Jennifer Louis, Jake Bejarano. Dr. Martin (Mentor), Dr. Gilley (Collaborator)

The gut community of the adult honeybee is simple, dominated by only nine bacterial taxonomic groups. We used this to characterize Bee-gut microbiomes with small set of real-time PCR quantifications. The PCR primers were three species-specific and two genus-level primer sets. Bees from a single hive were stored frozen, spring 2019. We purified DNA from abdomen contents collected after surface-decontamination. We calculated the relative abundance of the five taxonomic groups by a delta-delta Ct method modified from approaches common in gene expression studies. We measured the reference Ct with bacterial universal primers (V2V3) so that relative abundance is percent of total genomic ribosomal operons. Our previous work had showed very high levels of variability for Bees from a single hive. We have modified the surface decontamination protocol to limit exposure to bleach and now are purifying Bee-gut bacterial DNA in much higher quantities with much greater consistency for similar Bees collected at a single time-point from a single hive. These improvements should help us to better characterize Bee-colony responses to stressors.



## Characterization of New Cryptochromes in the Dinoflagellate *Karenia brevis*



**Alan Abboud and Dr. Emily A. Monroe (Mentor).**

*Karenia brevis* is a photosynthetic dinoflagellate responsible for the annual red tides in the Gulf of Mexico causing extensive marine life mortalities and human illnesses. We have previously identified new blue-light photoreceptor sequences in addition to *K. brevis*' cryptochrome DASH protein. To characterize the new photoreceptors, we will examine mRNA expression throughout the diel cycle and determine if their expression is under circadian control. Primers were designed for the top cryptochrome candidates showing the strongest homology to cryptochromes 1 & 2 in *Arabidopsis thaliana* and for the published *K. brevis* cryptochrome DASH sequence. Primer optimization was performed on *K. brevis* cDNA. We were able to amplify the product of interest for one cryptochrome candidate at an annealing temperature of 62 °C, and we are continuing to optimize the remaining primers. Characterizing new photoreceptors will help in understanding *K. brevis*' cell cycle and possible control mechanisms of bloom proliferation.

## **Testing the Transcriptional Disruption Resulting from Integration of Two Reporter Constructs at the MPP10-YJR003C Genomic Locus on Chromosome XII in Budding Yeast**



**Sarah Elkamhawy, James Arnone, PhD (Mentor).**

In our previously published study, we found that functionally clustered genes tend to localize to more transcriptionally permissive genomic loci when compared to singletons. Taking into account our previous findings, in this study I hypothesize that clustered genes are more likely to be transcriptionally disrupted upon integration of a reporter when compared to un-clustered singleton genes. In order to test this theory, I will be experimentally characterizing two mutant yeast strains, one of which will contain a KAN-URA3 highly expressed constitutively active reporter, while the second strain will contain an inducible *LEU2* reporter on the clustered region of the MPP10-MRX12 RRB gene pair. Through quantitative, real-time PCR I will observe the levels of disruption on the gene pair and the genes flanking this pair. In order to measure the efficiencies of the primers a Q-PCR was performed. The primers were found to be efficient in binding to their specific sequences, with efficiencies ranging from 90-113%. These findings permit the continuation of this study, where the characterization of the two mutant strains will be performed.

## Mechanism of Tail Resorption in Anuran Tadpoles



Ma. Veronica Holganza and *Jaishri Menon*\*

One of the most striking features in anuran metamorphosis is complete regression of the tail, in which reactive oxygen species (ROS) have a crucial role. Mitochondria and peroxisomes play a key role in ROS production and scavenging. ROS also affects mitochondrial transmembrane potential, which in turn opens mitochondrial permeability transition pathway (mPTP), resulting in halt of ATP synthesis, mitochondrial swelling, rupture, and cell death. In the present study, we performed *in situ* staining for ROS, peroxisomes, and mPTP in tail before and during metamorphic climax in tadpoles, *Xenopus laevis*.

Tadpoles at stages 60, 63 and 66 were stained *in situ* for ROS, peroxisomes and mPTP using kits from Molecular Probes (Life Technologies).

Confocal fluorescence microscopy has shown that later stages of metamorphosis is characterized by increased levels of ROS. Additionally, an increase in peroxisomal density is also observed as metamorphosis progressed. Areas of early cell death (such as ventral and dorsal fin), show increased ROS and peroxisome staining. mPTP staining showed an increased expression with the progress of metamorphosis.

Based on these observations, we conclude that one of the sources of ROS (responsible for cell death in tail regression) could be peroxisomes and increased oxidative stress leads to the opening of mitochondrial pores resulting in cell death.

## An inexpensive operant chamber that collects cognitive data 24/7

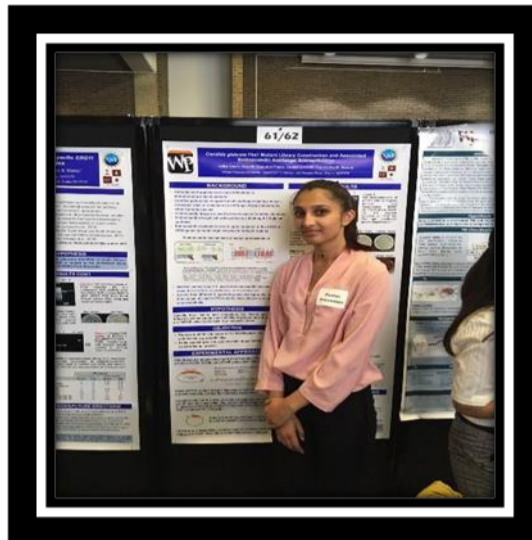


Jamie Carolyn Reulbach, David Freestone and Dr. Bierbower

### **Abstract:**

Finding the coefficient of variance (CV) of mice under specific circumstances is often the goal of interval timing experiments. Current proprietary operant chambers can collect cognitive data like the CV 24/7 using food reward systems, however these systems often cost hundreds to thousands of dollars and use niche programming languages. On top of the operant chamber expenses is the cost of specialized food pellets which can sometimes clog the system. Using the C57BL/6J strain of mouse bred at William Paterson University, we developed a cheap, DIY mouse operant chamber featuring a water reward system. Using the open-source electronics platform Arduino, we were able to program a timing procedure that transitions from a Fixed Interval (FI) task to a differential reinforcement of a low rate of behavior (DRL) task using simple C++ code. The new chambers still automatically gather cognitive data for a single mouse 24/7, are less than a tenth of the cost of the previous chambers, are easier to clean, do not require specialized food, and can be assembled in only a few hours.

**Determination of echinocandin antifungal susceptibilities following ectopic expression of medically relevant *FKS1* mutations in *Candida glabrata***



**Indira Sawh, Geselle Cancino-Prado, Cassie Girardin, Dr. K. Healey (Mentor).**

Invasive infections caused by the fungal pathogen *Candida glabrata* are treated with echinocandin antifungals. These semisynthetic lipopeptide drugs prevent fungal cell wall synthesis by targeting beta-1,3-glucan synthase, and resistance arises upon mutation of genes (*FKS1* or *FKS2*) that encode for the catalytic subunits of this target enzyme. To determine how specific *FKS1* mutations influence resistance levels within the same strain, several medically-relevant amino acid alterations (F625S, S629P, D632E) were incorporated into a plasmid carrying *FKS1* (pFKS1) through site-directed mutagenesis. Both *E. coli* (for propagation) and *C. glabrata*  $\Delta fks1$  were transformed with these plasmids. Transformants were screened by colony PCR and FK506 sensitivity to ensure proper pFKS1 presence and expression. Thus far, echinocandin susceptibility assays revealed 4-fold and 8- to 16-fold increases in minimum inhibitory concentrations upon expression of pFks1-F625S and pFks1-S629P, respectively, when compared to the plasmid carrying a wild type copy of *FKS1*. This experiment has provided the tools to test additional amino acid substitutions and analysis into how specific *FKS1* mutations influence drug resistance within an isogenic strain.

**Characterization of Gene Expression Pattern Changes in *Saccharomyces cerevisiae* as a Function of Genomic Distribution**



**Khizar Siddiqui, Reem Eldabagh\*, Dr. Jonathan J. Foley\*, IV, Dr. James T. Arnone (Mentor).**

Abstract:

Environmental changes elicit a response in gene expression to maintain cellular homeostasis and survival. Eukaryotic organisms cluster functionally related genes, coordinating transcription by adjacent gene correlation. Previous work in the budding yeast, *Saccharomyces cerevisiae*, identified 38 gene families with a statistically significant fraction of the composite member's clustered together, finding that 75% of these families have tighter transcriptional regulation throughout the cell cycle. To date, however, there has been no systematic characterization of this relationship in response to cellular stress. We analyzed the transcriptional responses in budding yeast, including heat shock and nutrient limitation, focusing on the role of spatial positioning and genomic distribution. We identified both and general and specific regulatory effects across multiple gene families. Our work identified general and specific patterns of regulation, such as the amino acid transport family, which has a varied response based on the stressor. Additionally, we have identified chromatin remodelers essential for this response.

## **Spider and Insect collection into taxonomy and information gathering**



**Marco Ortega, Mentor: Dr. J. Spagna**

### Abstract:

The goal of this research was to quantify the biodiversity of High Mountain Reserve focusing on the insects, and arachnids, particularly the spiders. Specific questions that were asked included: how many different types of arthropods are there, and what types of methods are most useful for capturing them? In June, July, and August, we hiked to High Mountain Reserve in Wayne, New Jersey every Wednesday during the evening, and Thursday during the night to collect the arthropod biodiversity. The collected specimens of that day were then identified; the arachnids were curated by storing them in labeled alcohol vials, while the hexapods and myriapods were pinned. Among arachnids, the common groups included Opiliones, commonly called harvestmen or daddy-longlegs, Araneidae (orb-weavers) and Lycosidae (wolf spiders). Insects included Rhaphidophoridae (cave crickets), Elateridae (click beetles), and Lampyridae (fireflies). The animals were most commonly found near tall patches of grass, near bundles of decaying vegetation, and on trees, specifically on the trunks and the crevices of the branches. Majority of the arachnids were captured roaming, but only a few were on their webs or in the process of building one. There were a total of 20 families of arachnids caught overall and 26 species. There were a total of 19 families of insects caught overall and 31 species. For the evening collection, there were 12 families of arachnids caught, and 15 families of insects caught. For the night collections there were 11 families of arachnids caught, and 9 families of insects caught. The best way to collect the insects was by aerial and ground nets during the evening. At night we used a black light to attract the insects and proceeded to capture them by hand or scooping them with the glass jar. As for the arachnids, we mainly collected them by hand. This is the second year of a multi-year arthropod survey. This sample was limited by time and could be improved by collecting in the fall when more arthropods are mature and easier to identify. We will be collecting more data that will aid in the tracking of the arthropods over time to see if there are changes in biodiversity and improve our understanding of how-to best sample them in the habitats around William Paterson University.

## Laboratory of Behavioral Genetics



Keimar Murray, Dr. J. W. Lee and Dr. Desroches

### Abstract:

There is a major importance for students involved in science to understand the opportunities they have without shying away due to the complexity. The goal of my internship was to gain the knowledge and understanding of these opportunities firsthand so I could encourage and inform other students about them in a way they will be able to acquire a profound understanding. With this, I hope to increase the amount of students actively participating in and taking advantage of the many research opportunities we have at the university.

Animal Labs are research facilities where typically mice and other species of animals are used as a means of furthering our understanding of many biological processes and diseases in order to develop means of treatment. Experiments of many designs are performed and rely on the practice of husbandry to ensure the overall health of the animals is well and the value of the data maintains its accuracy. It is important for lab technicians to be able to identify diseases and other health issues in each species of animal as well as taking steps to ensure the animals are not stressed as this can make results from experiments inaccurate. Professors conducting animal experiments rely on lab technicians to ensure the quality of data gained remains high.

In addition to learning these practices, I was able to become involved in and actively learn about the research projects of several professors who rely on the facility. I learned techniques and the types of experiments/studies done by several professors in the mouse lab including Dr. Lee's several studies with autistic mice, Dr. Onaivi's studies of endocannabinoid systems, Dr. Bierbower's studies of traumatic brain injuries, extending into several other professor's labs later on who do not rely on this facility to conduct research. After gaining these techniques and information I was able to put together informative documents regarding the research of these professors to ensure interested students had the opportunity to grasp and gain a profound understanding of these complex and amazing scientific studies.

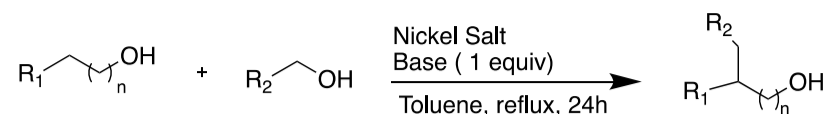
## William Paterson University, Chemistry Department

### Non-precious metal catalyzed direct synthesis of Guerbet alcohol



Emir Sehovic and Parminder Kaur (Mentor)

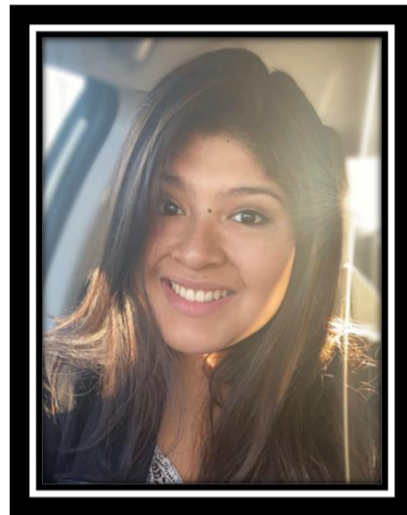
In the past decades, the development of transition metal catalyzed C-H functionalization boosted the scope of C-C and C-X bond formation reactions. This methodology requires the *in-situ* activation of the C-H bonds that results in the coupling leading to the formation of the desired product. In our current project, we are exploring the effect of non-precious nickel metal catalysts for the synthesis of Guerbet Alcohols, the reaction that involves the conversion of primary alcohols into the corresponding  $\beta$ -alkylated dimeric alcohol with the loss of water. The simple, inexpensive and readily available substrates make this an important and atom efficient reaction. A wide substrate scope of the reaction was demonstrated to prepare a wide variety of Guerbet alcohol derivatives. In this project, we are exploring the use of nickel and nickel-complexes for the cross-coupling reaction of primary alcohols for the direct synthesis of Guerbet Alcohols.



R<sub>1</sub> = Alkyl, Aryl, Heteroaryl  
R<sub>2</sub> = Aryl, Heteroaryl

### Proposed Mechanism:

Functionalization of C sp<sup>3</sup>-H Bonds via Copper Catalyzed Electrochemistry



Leslie Trigoura, Dr. Yalan Xing (Mentor).

Electrochemistry has made major contributions to organic synthesis through its “green” methodology, higher atom economy, and minimal waste. Organic electrosynthesis utilizes electrical current to drive the activation of organic molecules via the removal or addition of electrons. Due to its selective redox of organic molecules, organic electrosynthesis can perform reaction transformations that have not been generated traditionally through the use of conventional chemical reagents. Electrochemistry is a beneficial asset for chemists providing clean transformations, mild reaction conditions, simple scalability, high functional group tolerance, low energy consumption, and a step away from the use of toxic redox reagents. Through this research, we have developed a strategic electrochemical approach to perform this Csp<sup>3</sup>-H bond functionalization on C-H bonds adjacent to oxygen and nitrogen, using an undivided cell with graphite electrodes as both anode and cathode. The identification of the optimal conditions are currently under investigation in the laboratory.

### *De Novo* Approach Towards the Asymmetric Synthesis of Purpurosamine



Terrence Hopkins, Dr. George A. O'Doherty (Mentor).

The 2,6-diaminosugar, Purpurosamine C, is one of the two carbohydrate ring systems that make up the aminoglycoside antibiotic natural product Gentamicin C. As part of a study aimed at the discovery of new aminoglycoside antibiotic with lower toxicity and improved activity against resistant bacteria. We desired synthetic access to purpurosamine and its stereoisomers. To these ends, we have developed a *de novo* asymmetric synthetic approach to the purpurosamine ring system. The six-step asymmetric synthesis prepares either enantiomer of purpurosamine from the achiral starting material, *N*-Cbz-protected α-aminoacetyl furan. This new methodology starts with a Noyori catalyzed asymmetric reduction to install the D- or L-absolute stereochemistry. This was followed by a one-pot vanadium catalyzed peroxide mediated Achmatowicz rearrangement and *in situ* isocyanate annulation to form the desired pyran ring system with purpurosamine stereochemistry. A subsequent 4-step transformation, which involves the removal of a C-4 ketone, stereoselective glycoside formation and amine-deprotection provides the desired purpurosamine sugar.

## Ni/Cu-catalyzed oxidative C-H functionalization: Direct synthesis of allylic esters



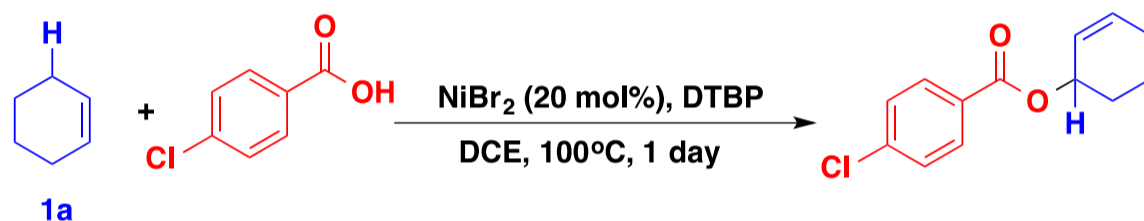
Jonathan McTague



Cassidy Anderson

Jonathan McTague, Cassidy Anderson and Dr. Parminder Kaur (Mentor).

In past years, research has been made in regard to transition metal catalyzed C-H functionalization, which has expanded upon the scope of various C-C, C-N, and C-O bond formation mechanisms. With such developments being made, transition metal catalysis offers the ability to potentially reform and improve upon previous synthetic methods. In this study, the efficacy of utilizing non-precious transition metal salts ( $\text{NiBr}_2$ ,  $\text{Ni}(\text{acac})_2$ ,  $\text{MnBr}_2$ ,  $\text{NiSO}_4$ ) to catalyze the synthesis of allylic esters via the oxidative coupling of allylic C-H and various substituted (H, Cl, F, Br,  $\text{CH}_3$ ,  $\text{OCH}_3$ ,  $\text{N}(\text{CH}_3)_2$ , OH) benzoic acids is observed. The resulting products are measured utilizing  $^1\text{H-NMR}$  to confirm the successful synthesis of the intended product. And it was observed that moderate to good yield of the product was obtained.



## Patterns in Protein Flexibility



Chris Reinknecht, Dr. David A. Snyder (Mentor).

Proteins are flexible macromolecules that perform a variety of tasks. Their (internal) motions can be simulated using MD (molecular dynamics) trajectories. While the results of MD simulations are generally consistent with experimentally derived measures of protein flexibility such as Lipari-Szabo order parameters and crystallographic B-factors, protein flexibility shown by MD simulations differs from the flexibility shown by B-factors in potentially critical ways. In particular, we find a pattern in backbone heavy atom flexibilities in superimposed MD trajectories, also found in coordinate uncertainties in superimposed NMR structures, but not typically found in crystallographic B-factors: namely, that amide nitrogen and carbonyl carbon coordinate variances tend to be smaller than  $\text{C}\alpha$  and especially carbonyl oxygen coordinate variances

### **Abstract for Dayanara Wert and Aya Matari, LSAMP Interns for Summer 2019**

The optical properties of multilayered nanostructures can be used to control thermal emission, which can increase the efficiency of a large number of devices and processes that rely on the conversion of thermal energy. This research focuses the optimization of multilayered nanostructures for controlling the thermal emission of visible light in incandescent light sources. We develop a methodology based on analytic gradients of luminous efficiency, a key figure of merit for incandescent sources, and implemented it in the software package WPTherml to accelerate the optimization filter structures for high luminous efficiency incandescent light sources. We have used this methodology to identify several structures with luminous efficiencies exceeding that of state-of-the-art LED bulbs. With continued research we can expand in identifying the overall most efficient structures by using their luminous efficiencies.

### **Publication Information resulting from LSAMP 2019 Work**

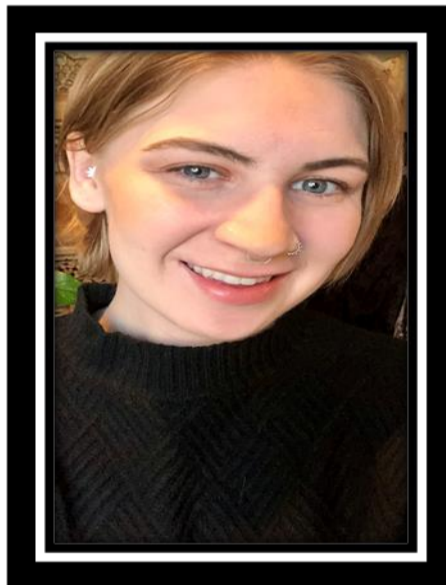
Title: Accelerating the discovery of multilayer nanostructures with analytic differentiation of the transfer matrix equations

Authors: James F. Varner, Dayanara Wert, Aya Matari, Raghad Nofal, and Jonathan J. Foley, IV

Journal: Physical Review Research, Volume: 2, Page: 013018, Year: 2020



### **Multi-Step Synthesis of the Natural Product Actinopolymorphol B**



Adriana Brandes, Maria Holganza, Alex Hildalgo, Claudia Kim, Chiara St Amant, Dr. Yalan Xing PhD (Mentor).

Actinopolymorphol A, B and C are a class of natural products isolated from a microorganism *Actinopolymorpha ritulus*. Our interest in Actinopolymorphol B stems from its hypothesized antimicrobial properties, although all three isolated molecules are still unknown in their biological mechanisms and effects. Currently our lab has been carrying out a multi-step synthesis of Actinopolymorphol B in order to study its medicinal properties in the future. This summer was focused on the final three steps in the total synthesis of Actinopolymorphol B after accumulating enough aldehyde intermediate to the starting molecule and proceeding with TMS acetylide anion addition.



## Optimizing the anti-reflective solar cell coatings by using the differentiation of the transfer matrix equations



Aya Matari, Dr. Jonathan Foley (Mentor)

Multilayered nanostructures speak to a significant class of materials with thermal radiative properties that can be utilized for a wide scope of energy applications. Specifically, this research seeks to develop a detailed understanding of the geometric parameters of the multilayers that compromise efficiency for the anti-reflective solar cell coatings, which have an important role to ensure that the overall transmission of the outside light is reached into the absorber region. Here we use a software package, developed by William Paterson university, known as WPTThermal as a theoretical system to optimize the geometry of such structures utilizing the gradients of different objective functions based on the differentiation of the transfer matrix equations. We exhibit the handiness of this technique by applying the matrix equations to design high-performance anti-reflection coatings for photovoltaic cells. PV conversion efficiency was tested by changing the thickness of AlN and SiO<sub>2</sub> stack layer with holding the Si layer fixed. The results demonstrate that effectiveness can be improved by changing the layer thickness when having the AlN and SiO<sub>2</sub> at 10,01 nm and 36.01 nm respectively.

## Synthesis of magnetic Iron Nanoparticles gels of *n*-(2-aminoethyl)-3-aminosilanetriol



Zoraya Perez, Qiaxian Johnson (Mentor), Dr. Bhanu P. S. Chauhan (Collaborator)

Iron nanoparticles have very potent magnetic and catalytic properties, therefore, they have great applications from medical imaging to the development of specific treatments for different diseases, such as breast and brain cancer.<sup>1</sup> One of the problems often encountered in terms of storage of iron nanoparticles is that due to their strong reactivity with oxygen in air and water, their oxidation and demagnetization takes place. Iron nanoparticles have been previously synthesized; however, the goal of our study is to stabilize iron nanoparticles with functional polymerizable silicon agents to create magnetic gels, where the magnetic particles are protected from oxidation and are stable and active. In this paper we will disclose that by employing the silane, *n*-(2-aminoethyl)-3-aminosilanetriol<sup>2</sup>, as stabilizing agents, iron nanoparticles were created which were stable and possess improved resistance to moisture and oxidation, while maintaining the nanoparticle magnetization.

Various analytical tools were used to conduct a thorough analysis of the resulting magnetic particles. Morphological analysis was carried out using TEM and SEM. Spectral characterization was carried out using FT-IR (Fourier Transform Infrared spectroscopy), NMR and UV-vis technologies. The TEM imaging analysis demonstrated that the iron particles are uniformly coated with 2-AST, and the presence of 2-AST was also confirmed by FT-IR. We will also disclose possible use of such nanoparticles for the development of new technological equipment and drug development.

- (1) Poller, J. M.; Zaloga, J.; Schreiber, E.; Unterweger, H.; Janko, C.; Radon, P.; Eberbeck, D.; Trahms, L.; Alexiou, C.; Friedrich, R. P. Selection of Potential Iron Oxide Nanoparticles for Breast Cancer Treatment Based on in Vitro Cytotoxicity and Cellular Uptake. *Int. J. Nanomedicine* **2017**, *12*, 3207–3220. <https://doi.org/10.2147/IJN.S132369>.
- (2) Chauhan, B. P. S.; Matam, S.; Johnson, Q. R.; Patel, A.; Moran, K.; Onyechi, B. Generation of Zerovalent Metal Core Nanoparticles Using N-(2-Aminoethyl)-3-Aminosilanetriol. *JoVE J. Vis. Exp.* **2016**, No. 108, e53507. <https://doi.org/10.3791/53507>.

## SOFTWARE METAPAPER

# WPTherml: A Python Package for the Design of Materials for Harnessing Heat

James F. Varner, Noor Eldabagh, Derek Volta, Reem Eldabagh and Jonathan J. Foley IV  
Department of Chemistry, William Paterson University, Wayne, NJ, US Corresponding author: Jonathan J. Foley IV  
(foleyj10@wpunj.edu)

WPTherml is a Python package for the design of materials with tailored optical and thermal properties for the vast number of energy applications where control of absorption and emission of radiation, or conversion of heat to radiation or vice versa, is paramount. The optical properties are treated within classical electrodynamics via the Transfer Matrix Method which rigorously solves Maxwell's equations for layered isotropic media. A flexible multilayer class connects rigorous electrodynamics properties to figures of merit for a variety of thermal applications, and facilitates extensions to other applications for greater reuse potential. WPTherml can be accessed at <https://github.com/FoleyLab/wptherml>.

**Keywords:** Nanophotonics; Solar Thermophotovoltaics; Passive Cooling; Radiative Cooling; Computational Electrodynamics; Concentrated Solar Power; Transfer Matrix Method

## (1) Overview

### Introduction

In 2017 over sixty five percent of energy produced was not useable and released as waste heat [1]; consequently, there are a large number of opportunities to develop technologies which can mitigate waste heat associated with energy production, including multi-layered nanostructure-based devices. Nanostructure emission properties are centrally important for many of these envisioned technologies, which include solar thermophotovoltaics (STPV) [2–4], radiative cooling devices [5], and highly efficient incandescent lighting [6] that minimize IR losses.

WPTherml (William Paterson University's tool for Thermal Energy and Radiation management with Multi-Layer nanostructures), is a computational engine for materials which can be leveraged for these and other technologies where the control of optical and/or thermal radiation properties is paramount. Specifically, WPTherml can be utilized to simulate optical properties (reflectivity, transmissivity, absorptivity, and emissivity) of nanostructures made from layered isotropic media; thermal radiation spectra of these nanostructures can be derived from these optical quantities in conjunction with Planck's blackbody radiation law. With these spectral quantities in hand, figures of merit for the design of such multi-layer nanostructures for applications such as STPV, passive radiative cooling, concentrated solar power, incandescent lighting, and plasmonics can be computed.

Thus, the WPTherml package serves as an engine for computing spectral quantities, and for relating these spectral quantities to relevant figures of merit. Central to the WPTherml package is a *multilayer* class; computation of spectral quantities and figures of merit are performed by methods of the *multilayer* class and are stored as attributes. Spectral quantities are computed within the framework of classical electrodynamics, specifically utilizing the transfer matrix method [7], which is implemented in a library called *tmm*. The required inputs for the transfer matrix method include the geometry (thickness) and refractive index of each layer in the multi-layer nanostructure, so the *multilayer* class has an associated method for parsing user input in an intuitive format to specify the geometry and material composition of a multi-layer structure. Refractive index data for a number of common materials is stored and accessed within a data library called *datatib*. This library also provides access to relevant data for the computation of various figures of merit, for example, spectral response functions of several popular photovoltaic materials (see **Figure 1** for an illustration of the spectral response of InGaAsSb), the AM1.5 solar spectrum, the photopic luminosity function, and the atmospheric transmissivity spectrum can all be accessed using the functionality of *datatib*.

The core of WPTherml is the transfer matrix method, implemented in the *tmm* library, which is a classical electrodynamics approach that relates the incident electromagnetic field upon a multi-layer structure to the reflected and transmitted electromagnetic fields, thereby permitting computation of reflection, transmission, and absorption of light by the multilayer:

# **William Paterson University, Environmental Studies Department**

## **Extinction of Iconic Megatoothed Shark *Otodus megalodon*: Preliminary Evidence from ‘Clumped’ Isotope Thermometry**



Chelesia Clarke, Allison Neumann, Shana Foster, Drew Pedersen, Troy Nixon, Clint Mautz, Dr. Michael Griffiths, Dr. Martin Becker, William Paterson University; Dr. Kenshu Shimada, DePaul University; Dr. Sora Kim, University of California Merced; Dr. Robert Eagle, University of California Los Angeles; Harry Maisch IV, The City University of New York.

The largest and most iconic extinct shark to have ever lived is *Otodus megalodon*. A general consensus indicates that the ability to thermoregulate in *O. megalodon* acted as a key driver for the evolution of gigantism that impacted its ecological role and success in surviving environmental changes. The cause for the extinction of *O. megalodon* is unknown, however it is hypothesized that the ability to thermoregulate played a role. In this study, shark teeth were drilled into a fine powder, acid washed, and sent to UCLA to be tested using Clumped Isotope Thermometry (CIT). CIT is a technique which relies on the thermodynamic preference of C13 and O18 to form bonds in the carbonate mineral lattice. These values can be used to determine body temperature of the animal while it was living and ultimately ability to thermoregulate

## ***Enchodus* from the Arkadelphia Formation-Midway Group Contact (K-Pg), Hot Spring County, Malvern, Arkansas: Implications for the effects of the K-Pg Mass Extinction Event on a Piscivorous Food Web**



Michaela Gardener, Mentor: Dr.M. Becker

A lag deposit between the Tocito Sandstone and Mulatto Tongue of the Upper Cretaceous Mancos Shale in Sandoval County, New Mexico, contains an assemblage of late Turonian–early Coniacian chondrichthyans and osteichthyans. This assemblage consists mainly of isolated teeth from at least 23 taxa. This lag was deposited along a series of sandbars in the San Juan Basin during global sea-level fluctuation in the late Turonian–early Coniacian. This sea-level event and concentration of specimens in a lag deposit is recorded in several other states within the Western Interior Seaway. These stratigraphic properties have correlative potential and provide a framework by which regional and eustatic sea-level events can be interpreted. Differences in coeval faunas found within these Turonian–Coniacian lags are bathymetrically controlled, related to the degree of taphonomic reworking and proximity of the ancestral shoreline.

9:00 – 10:15  
WELCOME & KEYNOTE ADDRESS

10:15 – 12:00  
POSTER SESSIONS

12:00 – 1:00  
LUNCH

1:00 – 1:30  
GRADUATE SCHOOL TALK

1:00 – 2:45  
TRANSFER & GRADUATE ADMISSIONS FAIRS

2:45 – 3:00  
POSTER AWARDS & CLOSING REMARKS

**11th Annual**  
GS-LSAMP/NNJ-B2B  
STEM Research  
Conference

Keynote Speaker  
TBD

**8 AM – 3 PM | Oct. 11, 2019**  
College Ave. Student Center, Rutgers – New Brunswick

REGISTER AT NOW  
[tinyurl.com/2019-GSLAMP-Annual-Conference](http://tinyurl.com/2019-GSLAMP-Annual-Conference)



**30+ ABSTRACTS AND POSTERS SUBMITTED**  
**the MOST from NJ**

**NEWSFLASH**  
Dr. Danielle Desroches, Biology Department  
GS-LSAMP- MAPS-BEC  
Coordinator and Advisor ,BMS Director ,  
SHE 4046 (973) 720-2329  
[d.desroches@wpsun.edu](mailto:d.desroches@wpsun.edu)  
<http://www.wpsun.edu/gslamp/>  
<http://www.wpsun.edu/gslamp/meeting-presentations/meetingseptember2014.dot>

**OCTOBER 11, 2019**

**Congratulations to GS-LSAMP students**

**AWARD WINNERS**  
**11<sup>TH</sup> ANNUAL GS-LSAMP CONFERENCE,**  
**RUTGERS UNIVERSITY**



Deeyana Wient (Chemistry, Dr. Foley)

Dora Euvodia (Biology, Dr. Barbowar)

Rosemary Arieta (Biology, Dr. Menon)

Elisa Maslam (Biology, Dr. Barbowar)

Adriana Brandes (Chemistry, Dr. King)

FLOR, EMALYN (Biology, Dr. Menon)

# 2019-2020 GS-LSAMP MONTHLY MEETINGS- STUDENTS PRESENTATIONS AND GUEST SPEAKERS



## PHOTOGRAPHS OF MONTHLY MEETINGS

Fall 2020







Spring Semester – Virtual Meetings

*Rutgers University 10th Annual GS-LSAMP STEM Research Conference - October 2019*



Save the Date!

**10th Annual  
GS-LSAMP  
Research  
Conference**

Friday, October 12, 2018  
8AM - 3PM  
College Avenue Student Center  
126 College Avenue  
New Brunswick, NJ 08901

Please join us for the 10<sup>th</sup> Annual Garden State –  
Low Stokes Alliance for Minority Participation/  
Northern New Jersey – Bridges to Bioinformatics  
STEM Research Conference

Keynote Speaker: TSA

To register, visit:  
<https://ajgo2018.gsamps.conference>

Keynote Address

Poster Presentations

Graduate School Fair

Poster Awards

**WPUNJ  
AWARD WINNERS  
10<sup>TH</sup> ANNUAL GS-LSAMP  
CONFERENCE, RUTGERS  
UNIVERSITY 2018**

**KRISTINA HAYEK, Environmental Sciences, Dr. M Becker, Mentor**  
**VERONICA MA MOLGANZA, Biology, Dr. J. Menon, Mentor**  
**LESLIE TRIGOURA, Chemistry, Dr. Y. Xing, Mentor**  
**MARIA KATRINA HOLGANZA, Biology, Dr. J. Arnone and Dr. Y. Xing, Mentors**





WILLIAM PATERSON UNIVERSITY OF NEW JERSEY

**WP**



**GS**

**LSAMP**

GS-LSAMP IS FUNDED BY A GRANT FROM THE NATIONAL SCIENCE  
FOUNDATION TO RUTGERS,  
THE STATE UNIVERSITY FOR THE ALLIANCE