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## **ROSE MERCADANTE SEMINAR SERIES**

**2022 Department of Chemistry and Biochemistry Undergraduate**

**Research Symposium**

**Book of Abstracts**

**December 13, 2022**

**Seminar: 5:45 – 6:45 PM  
Cristina Ventura Doctoral Presentation**

**Poster Session: 7:00 – 9:00 PM**

**Organizers:**

**Dr. Cosimo Antonacci  
Dr. Wyatt R. Murphy**

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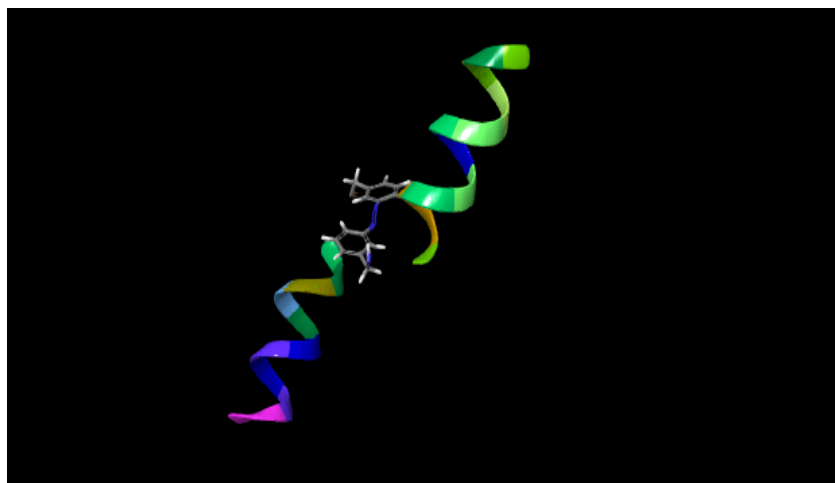
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## Doctoral Presentation

### PHOTOISOMERIZABLE MEMBRANE ACTIVE PEPTIDES

**Speaker: Cristina Ventura**  
**Mentor: Dr. Gregory Wiedman**

**Abstract:** Membrane active peptides (MAPs) interact with the cell membrane thus having a permeabilizing or translocating effect. Many alpha-helical membrane active peptides contain proline residues in the middle of their primary sequences. These proline residues break up the helix producing a helix-hinge-helix motif. Mutation of these proline residues have shown to have significant effects on the activity of the MAP. Azobenzene is a photo-switchable molecule that isomerizes from its *trans* to *cis* isomer upon excitation with ultraviolet (UV) light and from its *cis* to *trans* isomer upon excitation with visible light (VL). Substitution of proline for azobenzene preserves its hinge structure while adding the functionality of photo-switchability. In this work proline has been replaced in three distinct MAPs with an azobenzene amino acid. Azobenzene can be used to replace proline in MAPs that enables the activity of the peptides to be controlled with light. A 1.5-fold increase in activity was seen for UV treated photomelittin compared to the VL treated peptide. Conversely a 1.3-fold increase in activity was seen for VL treated photomaculatin 1.1 compared to the UV treated peptide. All the photoswitchable peptides retained their activity and the amino acid substitution did not change their mechanism of action. The peptides also exhibit new novel properties; peptide photobuforin II is fluorescent with an emission peak at 400 nm. This work provides a foundation for future studies optimizing azobenzene-containing membrane active peptides for uses in photopharmacology.



## Dr. Joseph Badillo

### **1. PHOTOACID GENERATORS AS CATALYSTS FOR THE CONJUGATE ADDITION OF INDOLES TO ALPHA-BETA UNSATURATED CARBONYLS**

Zena Salem, Alejandro Cubillos, and Joseph J. Badillo\*

Department of Chemistry & Biochemistry, Seton Hall University, 400 South Orange Ave, South Orange, NJ, USA



Photoacid generators are molecules that upon the absorption of light, produce strong acids. In general, photoacids have recently emerged as useful tools for a variety of synthetic reactions for pharmaceutical research. PAGs also have the added benefit of being air and bench stable before irradiation, which provides greater utility relative to air and moisture sensitive acids and Lewis acidic metals. This presentation will discuss the use of PAGs, such as triphenyl sulfonium triflate and nitro iodonium, as catalysts for the conjugate addition of indoles to alpha-beta unsaturated carbonyls. Reaction scope and optimization will be discussed, including the use of differently substituted indoles and carbonyls.

### **2. SYNTHESIS OF TRIAZOLE CONTAINING Bis(Indoyl)Methanes AND 3,3'-Di(Indoyl)oxindoles**

Evangelin Samuel, and Joseph J. Badillo\*

Department of Chemistry & Biochemistry, Seton Hall University, 400 South Orange Ave, South Orange, NJ, USA

The development of new catalytic processes is essential for organic synthesis. These reactions use a visible-light-induced, thiourea which catalyzes a C-C bond-forming reaction. Specifically, Schreiner's thiourea [(*N,N'*-bis[3,5-bis(trifluoromethyl)phenyl]-thiourea] functions as a photoacid to facilitate the double Friedel-Crafts addition of indoles to aldehydes and isatins to form the corresponding triarylmethanes and 3,3'-diaryloxindoles. From these parent compounds, triazoles will be synthesized using varying methodologies. In addition to this, a library of triazoles will be compiled by implementing click chemistry along with various azides.

### **3. SOLID SUPPORTED IRIIDIUM COMPLEX CATALYSTS IN PHOTOREDOX REACTIONS**

Jenna Mustafa, and Joseph J. Badillo\*

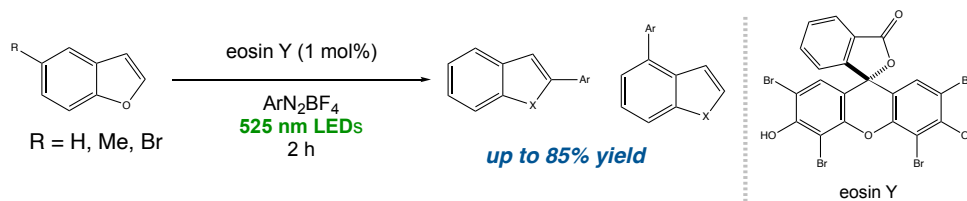
*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

In this experiment, we will test a reaction to merge photoredox with nickel catalysis. Photoredox catalysis involves a single-electron transfer. These catalysts are often transition-metals. (1; Electrochemical Series of Photocatalysts and Common Organic Compounds, n.d.) The reaction being tested is dicatalytic reaction, with a dicyclic process to create product. The first catalyst is Nickel Chloride and the second is an iridium photocatalyst complex synthesized at Seton Hall University by Dr. Murphy's Lab group. This reaction has been tested with several versions of the iridium complex. The aim of this project is to attach the iridium photocatalyst complex to a solid support. We chose to attach this catalyst to resin beads via peptide bonds. This is done at Seton Hall University by Dr. Weidman's Lab group. The catalyst is attached to these beads with the intention of retrieving these beads after the reaction in order to use them in subsequent reactions. Essentially, we mean to create a recyclable form of photocatalysis. We are working on using these catalysts in other photoredox reactions as well. We are testing carboxylic acids as activation groups for conjugate addition reactions.

## 4. PHOTOREDOX -CATALYZED MEERWEIN ARYLATION OF BENZOFURANS

Shreya Rawat, Karen Liu, and Joseph Badillo\*

Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079



In recent years, photoredox catalysis has emerged as a potent tool for molecular synthesis. The Meerwein arylation reaction, which involves the coupling of an aryldiazonium salt with an alkene, is often performed with the use of transition metals, bases, or palladium catalysts. The purpose of this project is to develop a photoredox-catalyzed Meerwein-type arylation with benzofurans and a variety of substituted aryl diazonium salts in order to synthesize 2-arylbenzofurans and 4-arylbenzofurans. The utilization of a catalytic-photoredox approach of this project possesses great significance as it enables the development of an alternative, energy-efficient reaction that proceeds at room temperature, eliminating the need for utilizing unsustainable compounds that the current methods necessitate. Our preliminary results have shown that some Meerwein-type arylation reactions, which were photoredox-catalyzed by Eosin Y, have rendered 2-arylbenzofurans and 4-arylbenzofurans in high yields. The regiomer ratio for these reactions is approximated to be 75:25, with the 2-arylbenzofurans forming at greater proportions than 4-arylbenzofurans. In order to analyze, isolate, and characterize our products, we have employed various techniques such as NMR spectroscopy, TLC, HPLC, column chromatography, X-ray crystallography, and chiral SCF. We plan to continue expanding the scope of this project by experimenting with a wider variety of substituted benzofurans and aryldiazonium salts, while also attempting to investigate more effective isolation and purification conditions.

## **Fr. Gerald Buonopane**

### **5. ANTIOXIDANT ACTIVITY IN PROLINE-LINOLENIC ACID MISTURES USING THE DPPH METHOD: INFLUENCE OF WATER ACTIVITY**

Aladeen Eewshah, Chisomo L. Gomodo, Ahmad Sheikh, Amber S. Chaudhary, Viral Shah and  
Rev. Gerald J. Buonopane\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange,  
New Jersey 07079*

Most processed and packaged foods often contain both a fat/lipid source and a protein/amino acid source. Fats can oxidize due to various environmental conditions, including elevated temperature and exposure to light. In particular, lipids that have oxidized can in turn react to oxidize amino acids and proteins within a food system. The resulting oxidized proteins are adversely affected in terms of their structure and function. Understanding the reactions of oxidizing lipids with proteins is important for determining reduction of nutritional quality of a food, as well as helping to predict quality deterioration during processing and storage. In this study, the amino acid proline and the polyunsaturated fatty acid linolenic acid were combined in model systems to study their interaction with one another at a temperature of 37°C for 7 days. It is noteworthy that proline has been shown to exhibit antioxidant properties. Antioxidant analysis employing the stable radical DPPH was used to determine oxidation of the fatty acid and possible antioxidant protection from the proline. Preliminary results show that proline has high antioxidant activity when used with linolenic acid, particularly at higher concentrations. The influence of water activity is also being considered in this study.

#### **References:**

<https://foodcrumbles.com/water-activity-in-food-the-theory/>

<https://thefooduntold.com/blog/food-science/water-activity-aw-and-food-safety/>



## **Dr. Jacob Goldsmith**

### **6. WHERE ART AND SCIENCE MEET: FIRST EXPERIMENTS ON MOCHA DIFFUSION**

Diana Malenkova, and Jacob Goldsmith\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Mocha diffusion is a ceramic surface decoration technique that is characterized by a dendritic pattern formation. It is presumed that the technique originated in the 18th century when potters accidentally spit chewing tobacco onto a clay slip, creating branching designs. Recipes were trade secrets, making it very difficult to explore the mechanisms of dendritic pattern formation. The technique involves chemical interactions between substances based on particle size, acidity, composition, gravity, zeta potential, and viscosity. Household, potter-available chemicals (such as apple cider vinegar, ethanol, water, soap, lemon juice, etc.) were utilized for the creation of oxide suspension mixtures. The pigments come from chemicals such as iron oxide black, rutile, copper oxide, cobalt blue, titanium oxide, and others. The current research design seeks to find an ideal combination of clay and dendritic slip in which a dendritic arrangement is prominent. Clay slip colloid is poured over a semi-dry test tile, and the acid-color mixture is applied dropwise on the surface to produce the design. After the pattern reaches an aesthetically pleasing dendrite, the test tile is fired in a kiln to cone 6 (or 1200°C) to ensure color retention in the formulation. Current research reports two formulations using iron (II, III) oxide and cobalt blue pigment that showed reproducibility and color preservation throughout the entire firing process.

Publicly available recipes were used for slip formulations. The set of experiments conducted explored oxide suspensions, various pH of the suspensions, the concentration of oxide in suspension, particle size in the slip, and the pre- & post-firing results. Results were obtained through morphological observations as well as diffusion radii measurements. A higher oxide loading was observed to produce more prominent, darker dendritic patterns. It was discerned that oxide suspensions that are too high in either acidic or basic content result in the loss of dendritic patterns and smaller diffusion radii. Particle size appeared to be an important factor limiting dendritic branching. Pre-fired and post-fired test tile results were compared to observe the effects of firing on the final color intensity. Firing produced different results for varying oxides-optimized iron oxide pattern lost nearly all coloration while cobalt blue became significantly more vibrant after firing. Although these two pigments yielded reproducible results, there are other color formulations to discover.

## Dr. Cecilia Marzabadi

### 7. THE SYNTHESIS OF A POTENTIAL ANTICONVULSANT DRUG

Leonarda Giannini, Dean Roundy, and Cecilia Marzabadi\*

Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079

In this project, studies have been done on a compound Deferiprone (3-hydroxy-1,2-dimethylpyridin-4-one) which is currently being used as a chelating agent for treating iron overload disorders. The goal of the project is to use a nitrogen analogue of a hexose sugar to create a compound that could potentially be effective in epilepsy treatment. Thus far, the protection of the hydroxide group on the molecule of Deferiprone has been carried out using a Williamson ether synthesis with benzyl bromide and sodium hydroxide. This is done first because the OH group is very reactive and can interfere in future reactions. Next, we will selectively reduce the ketone moiety, using a Luche reduction. Then the double bonds will be dihydroxylated. Finally, one of the vicinal diols will be protected as an acetal. The final product will be submitted for testing. Last semester, one of the most problematic things encountered was the loss of yield and a sample too small to continue to the next step after the Luche reduction.

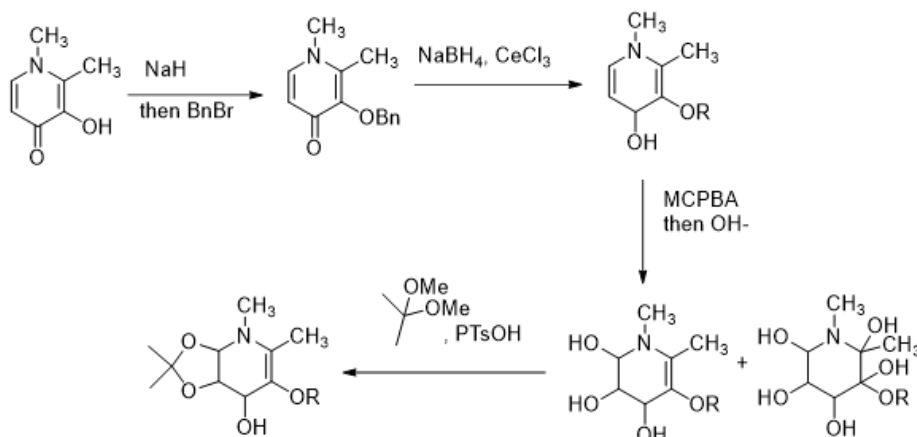


Figure 1. Reaction scheme

This semester, the focus was on optimizing the yield of the first reaction step by increasing the amounts of starting materials and by varying the benzylation reaction conditions and the purification of the benzylated product.

## Dr. Wyatt Murphy

### **8. GREEN SYNTHESIS AND CHARACTERIZATION OF [Ir(h-benzoquinoline)<sub>2</sub>(1,10-phenanthroline)]**

Josephine McCartney, Nataly Areosa , Allyson Dixon , and Wyatt R. Murphy Jr.\*  
*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Triplet oxygen ( $^3\text{O}_2$ ) can be catalyzed in conjunction with a photosensitizer to produce reactive oxygen species to be utilized in non-invasive treatment methods. This has formed the basis for Photodynamic Therapy (PDT), a new method aimed to treat a variety of diseases by utilizing the photophysical properties of light. Some compounds, including many iridium complexes, are reactive with light and produce singlet oxygen, a reactive oxygen species. Singlet oxygen is unstable and will destroy what is immediately surrounding it, making singlet oxygen producing compounds a target for antifungal or anticancer treatments. Compounds with photophysical properties and stability are of interest specifically those involving iridium(III) complexes with cyclometalating ligands such as h-benzoquinoline (bzq) and dative ligands like 1,10-phenanthroline (phen). Ir[(bzq)<sub>2</sub>(phen)] were synthesized using green microwave techniques<sup>1</sup>. These results will then be compared with other compounds produced to determine the most efficient compounds for Photodynamic Therapy and other applications. The compound synthesized, Ir[(bzq)<sub>2</sub>(phen)], yields promising results for applications within many different fields such as Photodynamic Therapy and Organic Light Emitting Diode (OLED) research. After establishing a concrete procedure using the microwave, lifetime, NMR, and quantum yield will be determined for the compound.

#### **References:**

1. Monos, T. M.; Sun, A. C.; McAtee, R. C.; Devery, J. J.; Stephenson, C. R. J. Microwave-Assisted Synthesis of Heteroleptic Ir(III)+ Polypyridyl Complexes. *J. Org. Chem.* 2016, 81 (16), 6988–6994. <https://doi.org/10.1021/acs.joc.6b00983>.

## **9. GREEN SYNTHESIS OF [Ir (bzq)<sub>2</sub> Dimethyl 2,2'-bipyridine-4,4'-dicarboxylate]**

Ishita Rana, Nataly Areosa, and Wyatt R. Murphy Jr.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Photodynamic therapy (PDT) is a non-invasive pharmaceutical technique which used light activated interactions of a specific wavelength between an iridium-based photosensitizer and molecular oxygen. This causes the rapid, local onset of vascular stasis and the eventual destruction of the wall of the target cells. It's capacity to control medication activity at a specified site and the production of cytotoxic singlet oxygen (ROS) are the basis for its medical usage. Using iridium (III) complexes offers multiple advantages including energy- level control, long lifetime, singlet absorption and large radiated quantum yields. Iridium (III) was used along side the cyclometallating ligand, h-benzoquinoline (bzq), and the dative ligand, 2,2'- bipyridine-4,4'-dicarboxylate (dicarboxy) to synthesize [Ir(bzq)<sub>2</sub>(2,2'- bipyridine-4,4'-dicarboxylate)]PF<sub>6</sub>. The groups' goal was to make the complex in high yield following the green chemistry initiative to ensure the preparation is completed in an environmentally friendly way. This method would also help reduce the overall reflux time with the use of the microwave because it would allow the reactions to be conducted in a significantly shorter period of time. After the synthesis of the complex, further examination was conducted including NMR, UV-Vis, lifetime, and quantum yield.

### **References:**

1. Jung Seung Nam, Myeong-Gyun Kang, Juhye Kang, Sun-Young Park, Shin Jung C. Lee, Hyun-Tak Kim, Jeong Kon Seo, Oh-Hoon Kwon, Mi Hee Lim, Hyun-Woo Rhee, and Tae-Hyuk Kwon. Endoplasmic Reticulum-Localized Iridium (III) Complexes as Efficient Photodynamic Therapy Agents via Protein Modifications *Journal of the American Chemical Society* 2016 138 (34), 10968-10977. DOI: 10.1021/jacs.6b05302

## **10. MICROWAVE ASSISTED SYNTHESIS AND PHOTOPHYSICAL ANALYSIS OF ROS GENERATING IRIIDIUM(III) COMPLEXES**

Josephine McCartney, Jyothi Maruthanal, Jessica Wasik, Elena Howe, Allyson Dixon and Wyatt R. Murphy Jr.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Photodynamic therapy (PDT) functions through the activation of a photosensitizer via light to generate reactive oxygen species (ROS). The ROS generating Iridium(III) complexes themselves can cause cell death and this is dangerous if not controlled. Thus, through tethering the ligand to a protein, this process can become target specific to kill particular diseased cells. The two compounds derived from this experiment were  $[\text{Ir}(\text{ppy})_2(4,4'\text{-dicarboxy-2,2'-bipyridine})]\text{Cl}$  and  $[\text{Ir}(\text{2phenylquinoline})_2(\text{bathocuproine})]\text{Cl}$ . To synthesize these compounds, microwave heating was utilized in order to increase the efficiency and purity of the compound. Through further experimentation, the intent is to measure values such as absorption maxima, molar absorptivity, radiative quantum yield, radiative lifetime, and oxygen quenching rate. The lifetime and quantum yield can be used to assess the efficiency of each compound at producing ROS, while the molar absorptivity is used to ensure the ability to determine the concentration of the compound in solution. The quantum yield enables us to see a measurement of how well the compound emits the photons. Additionally, the lifetime of a compound that produces ROS determines how long a compound is able to react with its surroundings and remain in its excited state. This permits us to ascertain how much ROS can be produced with our compound. The intent is to later take the compounds and run COrelated SpectroscopY (COSY) scans through the utilization of NMR processing which will allow us to determine whether the correct proton coupling groups were formed. This scan will help establish where the compound should be connected to on the protein. The proposed application of these compounds is the coupling to these proteins in order to destroy the diseased cells. By continuing to create compounds and analyzing their important mathematical values, we would be able to determine which ROS generating compound is the most efficient in this process.

## **11. SYNTHESIS AND CHARACTERIZATION OF SIX-MEMBERED RING SYSTEMS OF IRIIDIUM(III)**

Daniela Moncada, Nataly Areosa, Allyson Dixon and Wyatt R. Murphy Jr.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Organic Light Emitting Diodes (OLEDs) are electronic devices that employ a series of thin, light emitting films composed of various heavy metal complexes found in cell phones, televisions and computer screens<sup>1</sup>. One group of metal complexes used are cyclometalated complexes of iridium<sup>2</sup>. These complexes have a traditional dative bond and a bond to an anionic carbon. These ligands are indicated by C<sup>^</sup>N such iridium complexes can involve three cyclometalated ligands or two cyclometalated ligands, a dative ligand (N<sup>^</sup>N) using nitrogen donor atoms. In our research group, significant progress has been made in the greener synthesis of such complexes utilizing microwave heating. As such complexes are widely used in cell phone screens, lowering environmental impact of preparing these complexes by using less energy and enhancing the atom economy of the reaction methodology will have significant societal benefits. New cyclometalated iridium complexes with either blue or red emission of high efficiency are sought to improve OLED displays. We proposed to investigate two dative ligands not previously tested for OLED applications – 2-dipyridyl ketone and 2-dipyridyl methane. The goal of the research was to prepare the compounds in high yield to determine the purity of the compound as well as atom economy. Throughout the investigation there were different conclusions that were drawn for the 2-dipyridyl ketone and its properties, the most important of those being that 2-dipyridylketone does have viability for OLED application.

### **References**

1. Beeby, A.; Bettington, S.; Samuel, I. D. W.; Wang, Z. Tuning the Emission of Cyclometalated Iridium Complexes by Simple Ligand Modification. *J. Mater. Chem.* **2003**, *13* (1), 80–83. <https://doi.org/10.1039/B207502D>.
2. Flamigni, L.; Barbieri, A.; Sabatini, C.; Ventura, B.; Barigelletti, F. Photochemistry and Photophysics of Coordination Compounds: Iridium. In *Photochemistry and Photophysics of Coordination Compounds II*; Balzani, V., Campagna, S., Eds.; Springer Berlin Heidelberg: Berlin, Heidelberg, 2007; pp 143–203. [https://doi.org/10.1007/128\\_2007\\_131](https://doi.org/10.1007/128_2007_131).

## **12. MICROWAVE ASSISTED SYNTHESIS AND PHOTOPHYSICAL ANALYSIS OF [Ir(BZQ)<sub>2</sub>neo]PF<sub>6</sub>**

Evan Stull, Jyothi Maruthanal and Wyatt R. Murphy Jr.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Photodynamic therapy (PDT) is a process utilizing light in order to activate a photosensitizer to produce a reactive oxygen species (ROS), in turn eliciting cell death. A myriad of ligands have been bonded to iridium metal to learn different photophysical characteristics to determine which heteroleptic iridium complex proves to be best suited for PDT. The current complex under investigation is [Ir(BZQ)<sub>2</sub>neo]PF<sub>6</sub> due to its observed characteristic as an efficient emitter displayed by its lifetime and intensity of color within OLED studies. Thus, this complex has the potential to be a good PDT complex based on its similar characteristics as other complexes. The one-pot CEM microwave synthesis used to create this complex allows for a green and efficient reaction with a relatively fair yield. Molar absorptivity and emissions taken at 438 nm show promising results in comparison to known researched iridium complexes with respect to PDT. With further experimentation, the lifetime and quantum yield will be investigated to determine whether the compound is able to efficiently create an effective ROS.

## **13. TOPTIMIZATION OF THE GREEN SYNTHESIS OF CYCLOMETALATED COMPLEXES OF Iridium(III) WITH METHYL PHENANTHROLINES**

Roksana Najar, Allyson Dixon and Wyatt R. Murphy Jr.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Organic Light Emitting Diodes (OLEDs) and Light-Emitting Electrochemical Cells (LECs) have been studied and proven to have more advantages compared to semiconductor-based LED devices because of their energy efficiency and lower cost of production. The main emissive components of OLEDs and LECs are ionic transition metal complexes (iTMCs), specifically iridium (III) iTMCs (Ir-iTMCs). This work was built upon our previous work in which Ir-iTMCs containing neocuproine and bathocuproine respectively, were synthesized. Specifically, there was a strict focus upon a variation of dative ligands to improve our current synthetic methods to assess the impact of simple structural features on the photochemical properties of our complexes. The three dative (N<sup>^</sup>N) ligands that were studied were 1,10-phenanthroline (phen), 4-methyl-1,10-phenanthroline (4-Me-phen), and 5-methyl-1,10-phenanthroline (5-Me-phen). To broaden the range of Ir-iTMCs of the Murphy lab, these complexes were prepared with 2-phenylpyridine (ppy) and 2-phenylquinoline (pq) as cyclometalating ligands using microwave based green chemistry techniques. This paper will discuss the finetuned photophysical properties of 6 different cyclometalated complexes by either derivatizing one or both cyclometalating or dative ligands on which the HOMO and LUMOs reside, respectively.

## **Dr. Nicholas Snow and Dr. Wyatt Muphy**

### **14. ANALYSIS OF ALGAL-BASED BIODIESEL BY GAS CHROMATOGRAPHY AND MASS SPECTROSCOPY**

Natalie Mathews, Nicholas Snow\* and Wyatt R. Murphy Jr.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Biodiesels are composed of fatty acid methyl esters or fatty acid ethyl esters. These can be derived from plants, and in the case of this report, algae. This paper will primarily explore the analysis of algal-based biodiesels that have been produced from the species *Chlorella Vulgaris*. It will also briefly include the analysis of biodiesels from corn oil. Biodiesel is produced through a process known as transesterification. The analysis of this plant-derived fuel source is done through gas chromatography. This allows for the identification of the components that create biodiesel. The analysis and identification are done through gas chromatography. These components can then be analyzed further for the purposes of procedural development.

### **15. QUALTITATIVE ANALYSIS OF BIODIESEL FUEL SAMPLES BY GAS CHROMATOGRAPHY AND MASS SPECTROSCOPY**

Ria Sandeep, Nicholas Snow\* and Wyatt R. Murphy Jr.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Gas Chromatography is used as a separation technique in which substances partition between the stationary phase in the column and the mobile phase. Gas Chromatography-Mass Spectrometry serves as a method to separate components of a mixture, and then we can investigate the structures of those components using mass spectrometry. In this work, we use GC-MS on biodiesel fuel samples to characterize the diesel and gasoline components in order to determine its purity and conversion efficiency. The expected components of the biodiesel analyte are long chains fatty acids with 20-23 carbons. By using gas chromatography to analyze the biodiesel samples, we can test the hypothesis that the samples with the smaller content are the hypothesized biodiesel vials, and the ones with the larger content are hypothesized to contain an emulsion of unreacted oil and glycerin. In addition, we can compare the samples to previous work done with the biodiesel analysis and use the carbon chain chromatograms as a reference point.



## **Dr. Gregory Wiedman**

### **16. MICROWAVE COMPARATIVE ANALYSIS OF ATCUN WARHEAD VIRAL PEPTIDE AND TARGETING PEPTIDE ORGANOMETALLIC COMPOUND TO INFECTIVITY OF MURINE HEPATITIS VIRUS A59(MHV-A59)**

Makayla Manfredi and Gregory Wiedman.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Murine hepatitis virus A59 (MHV-A59) is a pseudovirus to severe acute respiratory-associated coronavirus 2 (SARS-CoV-2) with common structural features in their viral spike (S) glycoproteins. Areas based on non-heptad repeat regions with a high propensity to interact with the lipid interface of membranes play a vital role in novel approaches to identify new peptide inhibitors. Viral fusion proteins target cell membrane interactions and therefore could be targets for therapeutic interference. There are two potential methodologies that were tested and studied to disrupt these attachments. One is the combination of a redox active ATCUN warhead complex and viral peptide inhibitors that may interact with the cell membrane and copper ions to generate continuous reactive oxygen species (ROS), singlet oxygen. ATCUN motif sequences consist of all-amino acid components which are more cost effective and possess similar attributes to other ROS generating complexes such as iridium ligands. Two is the combination of a targeting peptide and organometallic photosensitizer that with the help of a specific wavelength will generate ROS. The photosensitization process where the transfer of energy excitation from ground-state oxygen to singlet oxygen, is an important aspect in oxidative degradation reactions. This process is the basis of photodynamic therapy that utilizes light, a sensitizer, and singlet oxygen to initial cell death. This discussion focuses on the comparison of ROS generating complexes such as iridium and redox active warhead ATCUN motifs.

## **17. MICROWAVE SYNTHESIS AND CHARACTERIZATION OF A CRYPTOCOCCAL ANTIFUNGAL PEPTIDE**

Zena Karam, Reesha Hora, Ishan Sharma, Miryam Kikhwa, Cristina Ventura and Gregory Wiedman.\*

*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange, New Jersey 07079*

Continuing last semester's antifungal studies, elements of the CDC50 loop region in fungal pathogen *C. neoformans* were once again used to develop a series of flippase inhibitors to be used and tested as microbial agents. After identifying the relevant biophysical properties of the peptides previously synthesized, the students determined all 15 AA long sequences in the CDC50 loop which are similar to the original in terms of hydrophobicity, net charge and isoelectric point. It is hypothesized that the peptides with the most similar properties will be the ones which behave most similarly. Solid phase peptide synthesis was used to synthesize the 15 amino acid long peptides, beginning with the furthest sequence away from the original, labeled QY-15ii. Mass spectroscopy and High-Performance Liquid Chromatography were used to analyze the detection and isolation of the peptide respectively. M+2H and M+3H peaks were found on the mass spectrum after the isolation of peptide fractions on the HPLC confirming the detection and isolation of the synthesized peptide. In future work, myristic acid will be added to the N-terminus of a peptide with the same amino acid sequence and will be also applied to analyze its effect as an antimicrobial peptide.

### **References:**

1. Tancer, Robert, "Flippase Inhibitors as Antimicrobial Agents" (2022). *Seton Hall University Dissertations and Theses (ETDs)*. 2981.  
<https://scholarship.shu.edu/dissertations/2981>

## **18. PROLINE SUBSTITUTIONS IN MEMBRANE ACTIVE PEPTIDES USING SOLID PHASE PEPTIDE SYNTHESIS**

Yogarupa Das, Siya Patel, Cristina Ventura, Akilah Mateen and Gregory Wiedman.\*  
*Seton Hall University, Department of Chemistry and Biochemistry, 400 South Orange Ave, South Orange,  
New Jersey 07079*

As a continuation of amino acid substitutions in order to determine different functionalities, our group was determined to learn about the substitution of proline. After finding several amino acids sequence relevant to the labs' purposes, the students substituted the organically found proline amino acids and substituted them with hydroxyproline, a common amino acid in bee venom. This amino acid typically contains anti-bacterial, anti-fungal, and antimicrobial properties, leading to our interest in overexpressing it in certain peptide sequences with hopes to increase these aspects. It was hypothesized that an increased expression of hydroxyproline would lead to more functionality of these environmentally helpful properties. After the research through prior articles, our group focused on the synthesis of Hydroxyproline Melittin, Hydroxyproline Maculatin, and Hydroxyproline Buforin. Solid-phase peptide synthesis was used to create these three peptides of interest, with the replacement of proline with hydroxyproline as it appeared in the amino acid. Mass spectroscopy and High-Performance Liquid Chromatography were used to analyze the detection and isolation of the peptide respectively. While running this examination, we were able to find multiple peaks that were relatively similar to what was expected for the peptides. In the future, we hope to synthesize a larger quantity of all three peptides in order to create a more definitive peptide in order to receive more accurate data. While our group only started with three peptides, we hope to expand to more proline-based peptides in order to run more diverse amounts of microbiological work on the peptides in order to assess their effects as an antimicrobial peptide.