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ROSE MERCADANTE SEMINAR SERIES

2023 Department of Chemistry and Biochemistry Undergraduate Research Symposium

Book of Abstracts

December 5, 2023

Seminar: 5:45 – 6:45 PM

Poster Session: 7:00 – 9:00 PM

Organizers:

Dr. Cosimo Antonacci

Dr. Wyatt R. Murphy

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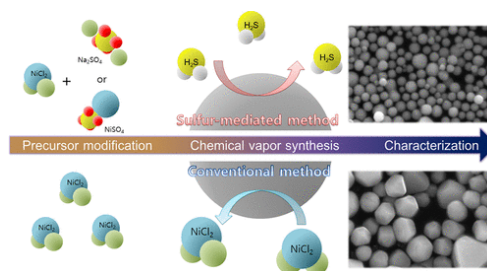
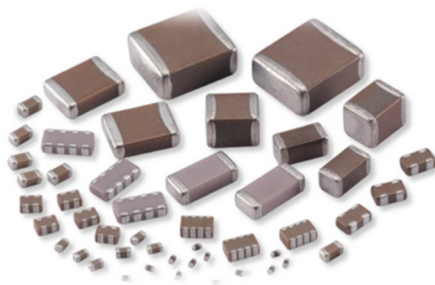
Formal Seminar Presentation

Nickel Nano-particles (Ni-NPs) in the manufacturing of Multi-layer Ceramic Capacitors (MLCCs)

(Formal Seminar)

Presenter: Vishal Parekh

Mentor: Dr. Nicholas H. Snow



Multi-layer ceramic capacitors are widely used passive components in electrical devices. They are made by stacking multiple alternate layers of ceramic dielectric and metal electrode. MLCCs temporarily charge and discharge to regulate the flow of current within the electrical device. They eliminate the noise and protect against device malfunction. Shrinking sizes with increased capacity of the electrical devices drive the demand for more sophisticated MLCCs with smaller sizes, higher capacitance, and reliable performance. Mass production and commercialization of Ni nano-powder with uniform size and shape is required for fabrication of internal electrodes in the form of thin sheets.

This research aims to use the Sulfur as dopant in the Nickel Chloride precursor to control the shape of nickel nanoparticles (Ni-NPs) prepared by chemical vapor synthesis. Spherical Ni-NPs were obtained when using anhydrous Nickel Chloride mixed with Nickel Sulfate or Sodium Sulfate with a molar ratio of 0.002 as precursors without changing any other process parameters whereas faceted Ni-NPs when using only anhydrous NiCl_2 as a precursor. First-principles calculations supported the experimental results, which showed that presence of Sulfur in the precursor favored the growth of spherical NPs.

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Dr. Joseph Badillo

Design, Synthesis, and Study of Second-Generation Photoacids

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In essence, our lab is trying to synthesize new catalysts with photophysical properties. Photoacid catalysts are an appealing area of research because of the flexible nature of photoacid architectures and the modularity of their photophysical properties. Photoacids are categorized as either a photoacid (PAH) or a photoacid generator (PAG). A PAH can undergo excited state proton transfer upon irradiation, become a strong acid, and return to its initial state. Meanwhile, photoacid generators (PAGs) irreversibly form strong acids resulting in the photodegradation of the parent compound. In previous years, Badillo's lab found that visible light-induced thiourea photoacids can facilitate C–C bond-forming reactions. Upon photoirradiation, Schreiner's thiourea (1) was able to catalyze the double Friedel-Craft's addition of indoles to aldehydes to form the corresponding triarylmethanes.¹ In 2020, Kokotos and partners showed that Schreiner's thiourea is capable of functioning as a photoacid catalyst for the formation of a diverse array of acetals derived from alkyl and aryl aldehydes.² In our goal to create a new photocatalyst, we looked at Schreiner's thiourea for reference to cultivate target molecules. Here we describe our preliminary results for the design, synthesis, and study of second-generation thiourea photoacids.

Fr. Gerald Buonopane

Water Activity of Selected Dry Foods and Oxidative Stability of Linolenic Acid-Proline Mixtures

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This study was carried out in two phases, first to determine the water activity of a variety of dry foods and second to assess oxidative stability of linolenic acid-proline mixtures using the DPPH method. It was anticipated that this research would lead to a further understanding of the relationship of chemical reaction rate (e.g., lipid oxidation) and water activity (a_w) in foods.

In the first phase, one set of dry foods was left out in weigh boats at room temperature; another set was stored in an oven at 37°C; and a third set was stored in a freezer at -14°C. The samples were held at their set temperature respectively for a total of 7 days with water activity measured on day 1, 3, 5, and 7 using a dew point water activity meter. The lipids from the samples were then extracted and tested via TBARS assays for a better assessment of their lipid oxidation reaction rates.

The second phase involved the determination of antioxidant activity in mixtures of fatty acid and proline in model systems. Studying the reactions of oxidizing lipids with proteins is important for predicting 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 stored at 37°C for 7 days. The second phase's preliminary results combined with the results of phase 1 provide interesting data toward establishing solid conclusions.

Dr. Nada Khan

Assessment of an Organic Laboratory Curriculum to Enhance Student Learning in Principles of Green Chemistry

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Green Chemistry is an ever-expanding discipline in the field of chemistry that has garnered much attention, especially in recent years. Chemical studies are integral to the development of scientific knowledge; however, these studies are also extremely costly. More specifically, educational centers across the world generate tons of chemical waste. Therefore, there is a growing demand for innovative scientific solutions that supply the necessary resources to further learning but also limit the damaging effects on the environment. This research hopes to find a solution by reforming the organic chemistry laboratory curriculum, starting with the Diels Alder reaction of anthracene-9-methanol with N-methylmaleimide. As part of this work, a revised organic chemistry lab protocol will be prepared which promotes the Green Chemistry initiative and assesses student learning of the tenets of Green Chemistry. As the Seton Hall University organic chemistry laboratory studies are conducted presently, many chemical wastes are generated. Ultimately, these reagents are transported to waste facilities and end up in landfills. Therefore, it is the mission of universities and educational centers to minimize their contribution of hazardous chemicals, while at the same time eliminating thousands of dollars in waste disposal costs. The following project works towards this mission.

Dr. Cecilia Marzabadi

Preparation of Sugar Diazene Adduct

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It has been found that glycals react with tetrazine in a Diels Alder reaction to form carbohydrate-based heterocycles. In this research, a large-scale reaction of 3,4,6-tri-O-acetyl-D-glucal was conducted with 1,4-carbomethoxytetrazine in toluene to produce a mixture of cycloadducts. The purification of the products from this reaction was performed by silica gel through column chromatography and preparative thin layer chromatography. With a clean product, it will be possible to perform further transformations of the cycloadducts.

Dr. Wyatt Murphy

GREEN SYNTHESIS AND CHARACTERIZATION OF [Ir(4,4-benzoquinoline)₂(1,10-phenanthroline)]

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Abstract:

Iridium complexes are ideal candidates for use within Organic Light Emitting Diodes, or OLEDs, due to their optimal photophysical properties and their stability. Ir(4,4-dimethoxyquinoxaline)₂(1,10-phenanthroline) was synthesized using green microwave techniques¹ although the ideal solvents and isolation techniques are still under investigation. This compound was synthesized from iridium(III) with 4,4-dimethoxyquinoxaline as the cyclometalating ligand and 1,10-phenanthroline as the dative ligand.

After establishing a microwave procedure, the lifetime, NMR, and quantum yield will be determined for the compound. These results will then be compared with other similar compounds synthesized to determine the most efficient compounds for use in OLEDs.

References:

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Microwave Assisted Synthesis and Analysis of Heteroleptic Iridium Complexes using Cyclometallating Benzo[h]quinoline

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Photodynamic therapy (PDT) is a novel, noninvasive treatment method for a variety of cancers. This alternative method is preferred in comparison to harsh treatments of cancer such as radiation or chemotherapy.¹ Although the research surrounding creating new complexes which can be used for PDT have typically been ruthenium-based due to its remarkable thermodynamic potentials and kinetic properties in electron transfer reactions,² many promising complexes have recently been formed using an iridium center. The benzo[h]quinoline ligand shows remarkable theoretical potential in the complex due to its rigidity, which is expected to restrict the vibrational relaxation of the complex in relation to its energy state, resulting in longer lifetimes and higher quantum yields.³ Current data for two complexes, [Ir(bzq)₂(neo)]PF₆ and [Ir(bzq)₂(batho)]PF₆ does not fully support this hypothesis, and so the veracity of this assumption and the data collected must be further scrutinized in order to fully verify the potential of benzo[h]quinoline as an effective cyclometallating ligand in PDT.

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Synthesis and Characterization of [Ir(2,3-diphenylquinoxaline)₂ 1,10-phenanthroline

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Since the original discovery of this unique bifunctional interaction, a rich chemistry of homo- and heteroleptic complexes of Ir(III) with cyclometalating ligands such as 2,3-diphenylquinoxaline involving simultaneous metal-nitrogen and metal-carbon bonds has advanced. Substituted quinoxalines are known building blocks for compounds with pharmacological, agricultural, and material uses. Phenq can undergo nucleophilic aromatic substitution however it must be in the presence of metal catalysts. This research focuses on a robust microwave-assisted one-pot procedure to gain efficient access to [Ir(2,3-diphenylquinoxaline)₂ 1,10-phenanthroline]. Once synthesized, further examination was conducted which included UV-Vis, quantum yield, lifetime, and NMR.

Dr. Reihaneh Safavisohi

Exploring Transmembrane Proteins: Small and Large Extracellular Vesicles from Colon Cancer Cell Lines

Savannah Nembhard and Dr. Reihaneh Safavisohi*

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Cells can communicate with neighboring cells or distant cells through extracellular vesicles (EVs). EVs are heterogeneous and display a diverse range of sizes (50–200 nm in diameter). These EVs are composed of a lipid bilayer containing transmembrane proteins and enclosing cytosolic proteins. Transmembrane proteins are proteins that have inserted or anchored themselves into or to a targeted membrane via translocons (1). Transmembrane proteins allow for ions diffusion across their associated membrane. They trigger immune, hormonal and neurological responses in signaling pathways, deliver essential nutrients, and play a crucial role in cell-cell communication (2).

In this study, we focused on transmembrane proteins in order to explore quantitative proteomics data from colon cancer cell lines. Transmembrane proteins were extracted from the data set and were sorted according to their protein class using previously published quantitative proteomics data (3). Extraction and classification of transmembrane proteins were performed on a dataset of 2421 proteins, identifying 358 proteins significantly differing between small and large EVs. Of these, 133 were recognized as transmembrane proteins, with four associated with large extracellular vesicles (LEV) and the remaining 129 with small extracellular vesicles (SEV).

A total of 9 peripheral proteins were detected among 133 transmembrane proteins. Overlapping functions were observed in the dataset, with a limited number being unique. To facilitate understanding of differences and commonalities, pie charts, violin plots, and data tables were employed for visualization. Considering their versatile functions, transmembrane proteins are promising candidates for drug delivery and warrant further investigation into their mechanisms of action.

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Dr. Nicholas Snow

Analysis of Active Pharmaceutical Ingredient (API) Acetaminophen Using Gas Chromatography with Flame Ionization Detection (GC-FID)

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Pharmaceutical products contain various Active Pharmaceutical Ingredients (APIs) in fixed portions that participate in the treatment of specific ailments. High-Pressure Liquid Chromatography (HP-LC) has historically been used as the preferred analysis method for APIs over Gas Chromatography (GC). This is generally due to the associated limitations of column technology. Gas Chromatography theory was initially developed using packed columns. This restricted analysis to highly volatile, non-polar compounds with lower boiling points, so as to not exceed the maximum temperature of the column or system. With many APIs being polar in nature, the likelihood of analyte degradation is increased because their boiling points are well above possible working conditions for analysis via Gas Chromatography. Advancements in column technology, specifically capillary columns, using High-Temperature Gas Chromatography for the API Acetaminophen is revisited in this work.

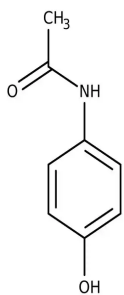


Figure 1: Acetaminophen



Figure 2: The Lucidity mini-GC

A method for the analysis of Acetaminophen using GC-FID was developed and demonstrated that elution and analysis of a compound with a high boiling point is possible. This is possible because capillary columns allow for APIs, such as Acetaminophen, to elute far below their boiling points by prioritizing differences in vapor pressure to be the driving force. Gas Chromatography column technology has evolved to make GC a greener alternative to LC for the analysis of APIs. One of the ways this work seeks to achieve this is through miniaturization of the machines used, namely the Lucidity mini-GC, which has a smaller footprint compared to machines such as the Shimadzu Nexis GC-2030.

Dr. Gregory Wiedman

SYNTHESIS AND CHARACTERIZATION OF AZOBENZENE MOIETY WITH TYROSINE

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In previous studies, it has been shown that azobenzene has a special property to isomerize with light. In conjugation with an aromatic amino acid, namely tryptophan, it showed fluorescence at 365 nm. In this study, it was hypothesized that a peptide consisting of the conjugation between azobenzene and tyrosine will present similar photochemical properties and possibly fluoresce due to tyrosine's aromatic nature. A peptide was synthesized through solid phase peptide synthesis by coupling azobenzene to pre-loaded tyrosine resin beads. Analytical High-Performance Liquid Chromatography was used to confirm the presence of both tyrosine and azobenzene in the peptide. When placed under 365 nm ultraviolet light, the peptide appeared not to fluoresce distinctly as shown with the azobenzene-tryptophan peptide. In future studies, synthesis of several separate peptides consisting of individual combinations of differently synthesized azobenzene moieties and aromatic amino acids can be focused on for reproducible and repeatable results determining the effects of aromatic amino acids in conjugation with azobenzene.

References:

Frederic, Charnette, and Gregory R. Wiedman. "Investigating the interaction of azobenzene moiety on the aromatic amino acid tryptophan." *Peptide Science*, 2023,
<https://doi.org/10.1002/pep2.24334>

Conjugation of Anti-HER2 Affibody to a pH Sensitive Membrane Porating Peptide

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Affibodies mimic the properties of antibodies while only being 1/25th of the size (6kDa vs 150kDa). We attempted to conjugate anti-HER2 Affibodies synthesized by Dr. E. Szedlacsek (Institute of Biochemistry of the Romanian Academy) to pH sensitive peptides with membrane porating activity. We hypothesize that if conjugated, the peptide and affibody can function in tandem to selectively destroy HER2-positive cancer cells. This semester, we attempted to develop a method to conjugate the affibody and peptide based on pre-existing bioconjugation techniques, as well as an assay that can reliably confirm conjugation. Three methods were tested: Gel electrophoresis, UV-Vis spectrometry via NanoDrop, and mass spectrometry. While a precipitate was formed from the bioconjugation following incubation, neither the gel-based nor UV-Vis method has been demonstrated to determine conjugation.

MICROWAVE SYNTHESIS AND CHARACTERIZATION OF A CRYPTOCOCCAL ANTIFUNGAL PEPTIDE

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Continuing previous 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 antimicrobial agents. Several sequences in the CDC50 loop that are similar to the original in terms of hydrophobicity, net charge, and isoelectric point were generated after determining the pertinent biophysical properties of the peptides that had previously been synthesized. It is predicted that the peptides that behave most similarly will be those with the most similar properties. Solid phase peptide synthesis was used to synthesize the 15 amino acid long peptides, starting with QY-15ii, the sequence that differed the most from the original. High performance liquid chromatography was performed on our synthesized peptide. However, due to an error when reading the peaks, a new method is planned to be created in order to isolate and purify the proper peptide. Our future endeavors involve conducting a Microtiter Plate-based Minimum Inhibitory Concentration (MIC) assay on the peptide to comprehensively evaluate its anti-fungal properties. This meticulous analysis aims to ascertain the minimum concentration of the peptide required to inhibit the growth of fungal organisms, providing invaluable insights into its efficacy as a potential anti-fungal agent. The MIC assay will be executed with precision, employing standardized procedures to ensure the reliability and reproducibility of our findings. The outcome of this investigation will significantly contribute to our understanding of the peptide's therapeutic potential in combating fungal infections.