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Petersheim Academic Exposition

Petersheim Academic Exposition

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4-26-2022

## Book of Abstracts

Seton Hall University

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## **ROSE MERCADANTE SEMINAR SERIES**

**Department of Chemistry and Biochemistry**

**27<sup>th</sup> Departmental Symposium**

*in conjunction with*

**The Petersheim Academic Exposition**

**Book of Abstracts**

**Hybrid Poster Symposium**

**April 26 2022**

## **Foreword**

Over 25 years ago, Dr. Matthew Petersheim had the idea that each year there should be a time when the Academic Excellence of the University was celebrated. He believed that a time of focus on research and scholarship and a celebration of academic excellence was the least that could be done to reward those pursuing this central goal of Seton Hall University. The result of this idea was the Academic Exposition. After his untimely death in 1998, the Exposition was named in his honor. Each year, the Academic Exposition continues to reinforce Dr. Petersheim's vision.

The Department of Chemistry and Biochemistry has held a Research Symposium each year of the Petersheim Academic Exhibition. Dr. Petersheim was our colleague and Chair of the Department, so his vision of a celebration of research and scholarship is one that we share.

The past two years, the Academic Exposition has faced unique challenges. The epidemic due to COVID-19 has resulted in unforeseen changes in teaching, scholarship and research. The Department of Chemistry and Biochemistry has risen to meet these challenges, and this year we combine our traditional in-person poster session with a virtual poster session that allows those members of our community who can not attend in person to share in the celebration of scholarship. In this book, you will find Abstracts of all of the posters presented at the symposium, organized by research mentor. The online poster session can be found at the Chemistry Biochemistry Graduate Student Blackboard site, as a collection of Wikis, also organized by research Mentor.

Hazard Zet Forward!

Dr. James E. Hanson  
Director of Graduate Studies  
Department of Chemistry and Biochemistry  
Seton Hall University

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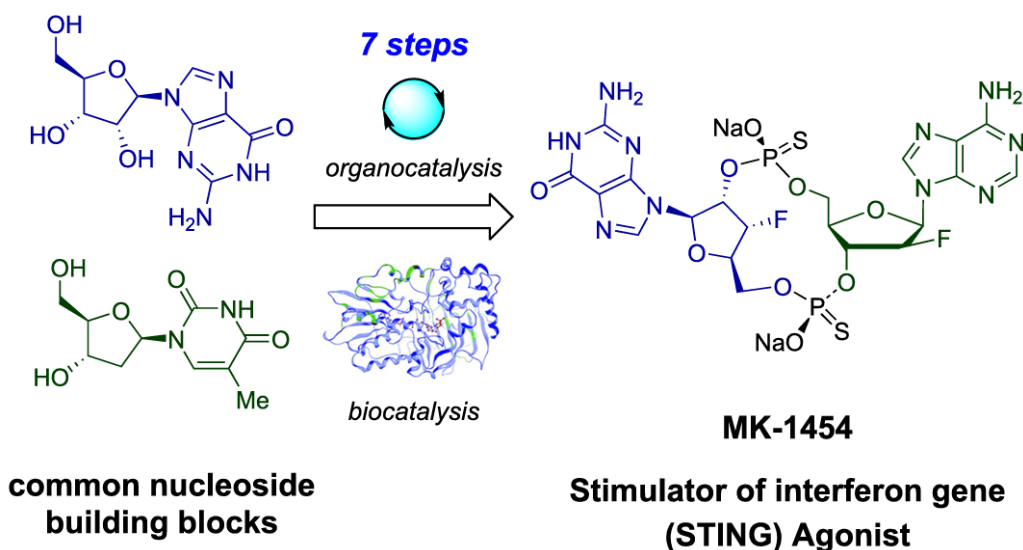
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## Keynote Presentation

Nastaran Salehi Marzijarani

### Accelerating Drug Development Through Innovation for the Stereoselective Synthesis of Cyclic Dinucleotide MK-1454

Over the past decades, Merck's Process R&D group has deemed greenness and sustainability as key attributes of ideal synthetic routes and has invested in a culture that strives to invent new chemistry and technologies in their pursuit. In the context of an immuno-oncology focused program, we identified the stereocontrolled synthesis of cyclic dinucleotides (CDNs) as a significant unsolved problem. Therefore, we developed a highly diastereoselective synthesis of MK-1454, a potent agonist of the stimulator of interferon gene (STING) signaling pathway. The synthesis begins with the asymmetric construction of two fluoride-bearing deoxynucleotides. The routes were designed for maximum convergency and selectivity, relying on the same benign electrophilic fluorinating reagent. From these complex subunits, four enzymes are used to construct the two bridging thiophosphates in a highly selective, high yielding cascade process. Overall, these developments and innovations led to vast reductions in PMI and substantial gains in sustainability, efficiency, and process safety.



## **Characterization of Immune Responses to Coronavirus Spike-Fc Fusion Proteins**

Ellora Haukenfrers, Lea Marjana\*, Lorena Pena\*, Dr. Cosimo Antonacci, Dr. Daniel Nichols\*,  
Dr. Constantine Bitsaktsis\*

Department of Chemistry and Biochemistry, *Seton Hall University*

\*Department of Biological Sciences, *Seton Hall University*

Despite the availability of several vaccines and antivirals, SARS-CoV-2 continues to represent a significant threat to the public health. The rise of several new variants of concerns highlights the need for continued research in immune responses against coronavirus infections. In this project, immune responses to coronavirus spike proteins fused to the Fc region of the IgG1 mouse immunoglobulin is ongoing. The S1 region of the spike protein from either SARS-CoV-2 or Murine Hepatitis Virus (MHV) A59 were cloned in a pFUSE expression plasmid inframe with mouse Fc. This vector was transformed into competent *E.coli* strain DH5alpha using zeocin as a selection marker. Individual colonies were isolated and cultured overnight and the pFUSE plasmid DNA is extracted using the PureYield™ Plasmid Miniprep System (Promega) and the concentration and purity of DNA is recorded using a nanodrop. Restriction enzymes EcoRI and NcoI are then applied to the plasmid in combination with the SARS-CoV-2 and MHV spike to be digested and a gel electrophoresis is performed to verify the presence of the Spike S1 inserts from the gel. To express and purify the Coronavirus Spike Fc fusions, Chinese hamster ovary (CHO) cells are transfected and plated down with varying antibiotic concentrations of both Zeocin to select for cells that have taken up the plasmid. . The pFUSE vector contains a zeocin resistance markers that allow isolation of transfected cells. Expression of SARS-CoV-2 Spike S1-Fc and MHV-A59-Spike S1-Fc is verified via immunoblotting Once enough protein has been produced, purification will be performed with the Pierce™ Chromatography Cartridge Protein G procedure for antibody purification using a syringe to extract the Fc-tagged spike proteins for characterization in a mouse model.

Brennan Isaac  
Dr. Antonacci, Dr. Hanson, and Usha Kalra

### Cationic Porphyrin via Click Chemistry

The preparation of cationic porphyrins is important for a variety of biochemical studies. The traditional method of alkylation of tetra-pyridylporphyrin is very inefficient, requiring very large excess of alkylating agents. The usage of “click chemistry” as an alternative method for the preparation of tetracationic porphyrins is explored instead. Azide-alkyne cycloaddition is the primary mechanism for the reaction and is useful for a wide range of products. Once purified, the cationic molecules will be used to bind G-quadruplex structures. The focus of these studies are to analyze conformational change, thermal stability, and binding affinity which could further expand the use of cationic porphyrins in targeted therapies.

**Title**

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

**Authors**

Nicholas DeFilippo, Alejandro Cubillos, Dr. Joseph Badillo

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

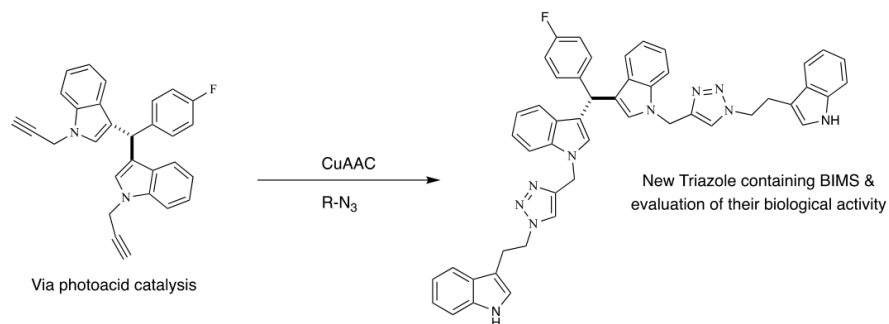
**Abstract**

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.

## Synthesis of Triazole Containing Bis(indolyl)methanes and 3,3'-Di(indolyl)oxindoles and Evaluation of their Biological Activity

Jason Saway, Evangelin Samuel, Ali Akram and Joseph Badillo\*

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

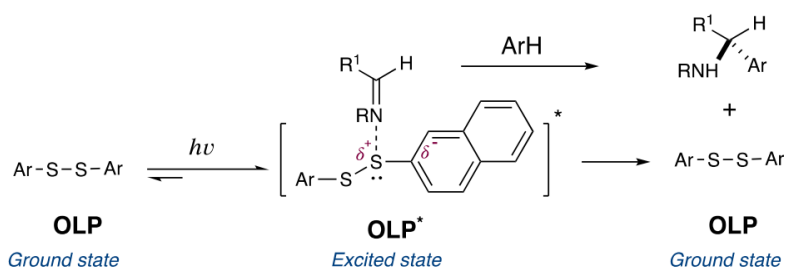


Our laboratory recently developed a mild photoactivated strategy for the synthesis of bis(indolyl)methanes and 3,3'-di(indolyl)oxindoles. Bis(indolyl)methanes (BIMs) are of interest due to their interesting anti-cancer properties. This presentation will discuss the synthesis of a variety of triazole containing BIMs and 3,3'-di(indolyl)oxindoles using copper-catalyzed azide-alkyne cycloaddition (CuAAC) chemistry. In collaboration with the Gantar Lab in the Department of Biological Sciences, preliminary evaluation of the biological activity for these triazole-containing compounds will also be discussed.

## Organo-Lewis Photoacid Catalyzed Synthesis of Amines

Andrea Serrano Trujillo and Joseph Badillo\*

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



This project focuses on the development of an organo-Lewis photoacid catalyst for the synthesis of amines from their corresponding imines. Upon irradiation, excited-state disulfide containing aromatics such as 1,2-di(naphthalen-2-yl)disulfane become potent Lewis acids that can be engaged in catalysis. In general, the use of photocatalysis provides a more environmentally benign method for organic synthesis complimenting previous methodologies for the synthesis of amines.

**Title**

Photoacid Catalyzed Acetalization of Carbonyl Compounds

**Authors**

Jason Saway, Abigail Pierre, Joseph J. Badillo

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

**Abstract**

We have shown that 6-bromo-2-naphthol (2) functions as a photoacid catalyst for the formation of a range of acetals and ketals. These acetal and ketal products serve as protecting groups enabling the synthesis of complex natural products and pharmaceuticals. NMR studies provide evidence for a hydrogen bonding complex between (2) and benzaldehyde, as indicated by a downfield shift and broadening of the hydroxyl peak of (2). Interestingly, the hydroxyl chemical shift after irradiation indicates increased H-bonding/formation of an in situ generated acidic species. In addition to these NMR studies, we also were able to determine both the ground state acidity ( $pK_a$ ) and excited-state acidity ( $pK_a^*$ ) for 2-naphthol (1) and (2). This was also the first time that the  $pK_a$  for (2) has been determined in water.

**References**

1. Salem, Z. M., Saway, J., & Badillo, J. J. Photoacid-Catalyzed Friedel-Crafts Arylation of Carbonyls. *Organic Letters*. 2019, 21, 8528-8532.
2. Saway, J., Salem, Z. M., & Badillo, J. J. Recent Advances in Photoacid Catalysis for Organic Synthesis. *Synthesis* 2021 (Vol. 53, Issue 3).



Authors: Viral Shah, Amarilis Rodriguez, and Dr. Gerald J. Buonopane,

SETON HALL UNIVERSITY, COLLEGE OF ART AND SCIENCES, CHEMISTRY  
AND BIOCHEMISTRY DEPARTMENTS

Abstract Title:

**THE 2,4-DINITROPHENYL HYDRAZINE REACTION WITH METHYL LINOLEATE  
NON-VOLATILE CARBONYLS OXIDATION PRODUCTS.**

Under various conditions, monounsaturated and di-unsaturated carbonyls are produced from methyl linoleate oxidation reactions. Carbonyls are considered secondary lipid oxidation products and are derivatized with 2,4-Dinitrophenyl hydrazine (DNPH) under acidic reaction conditions. DNPH derivatization is specific for secondary oxidation carbonyl products. In comparison, p-anisidine and thiobarbituric (TBA) acid derivatizations are not specific secondary oxidation carbonyl products.

Major carbonyl products are Decanal, Heptanal, Nonanal, and Octanal. Their solubility was evaluated in acetonitrile, Acetonitrile: water:70:30, and Dimethylformamide (DMF). The carbonyls were derivatized with DNPH under acidic conditions and used DMF as diluent. Hydrazones are analyzed using reverse-phase high-pressure liquid chromatography (RP-HPLC) with LC column Ultra C18 with a 2.1 mm internal diameter and an ultraviolet detector (UV) to detect. Hydrazones were separated in RP-HPLC and retention times (RT) of compounds were determined to demonstrate specificity and linearity. The correlation coefficient for regression curve, slope, y-intercept, and bias of linearity and range (0.008 to 0.6 mmol/L) were determined. These experiments were performed to establish a linearity and determine the range for different chain length hydrazones. Furthermore, to identify and quantitate non-volatile carbonyl oxidation products from methyl linoleate oxidation.

Authors: Viral Shah, Amarilis Rodriguez, and Dr. Gerald J. Buonopane,  
SETON HALL UNIVERSITY, COLLEGE OF ART AND SCIENCES, CHEMISTRY AND  
BIOCHEMISTRY DEPARTMENTS

**Abstract Title:**

A Study of Appearance and Conjugated Diene Formation, Accumulation, and Stability in Methyl Linoleate and Proline Dry Model Food Systems at Different Temperature Conditions

**Abstract:**

The formation of conjugated dienes was investigated in dry model food systems containing methyl linoleate (ML) and proline under various time and storage temperature conditions. Conjugated dienes are produced in initial stages of lipid oxidation. Different temperature conditions and amounts of proline present affected conjugated diene formation, accumulation, and stability in ML samples.

The ML molecule forms a radical to initiate oxidation by attacking an initiator on a double bond. The radical forms conjugated dienes (CD) by double bond shifting. ML oxidation rate is high in a dry sample matrix and at a high temperature. We evaluated ML and proline mixes (1:1, 1:5, and 1:10 moles) stored in the freezer, refrigerator, room temperature, 37°C, and 65°C for five days to analyze CD formation and examine sample appearance.

Measurements of the ultraviolet absorption spectra of the ML samples provide valuable information on conjugated double bonds. Three-mL iso-octane were added to the sample vials and vortexed. The samples with proline were centrifuged, and the supernatant solution was used for analysis. Sample solution UV profiles were obtained from 200 to 300 nm, and CD was measured at adsorbing UV 234 nm.

ML and proline mixed samples were not opaque and transparent from the second day at 37°C and 65°C compared to control ML. The appearances were not changed in control ML and control proline samples at all five temperatures from day zero to five days. Sample appearance and CD results remained the same in all samples at freezer and refrigerator temperatures. The CD concentration increased on the fifth day in M:P: 1:10 at room temperature. The results show CD accumulation increased over time at 37°C and stabilized up to the first day at 65°C in ML control samples. CDs are stabilized up to the third day at 37°C and up to the first day in ML and proline mix samples.

**Title**

Where Art and Science Meet: First Experiments on Mocha Diffusion

**Authors**

Diana Malenkova, Dr. Jacob Goldsmith

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

**Abstract**

Mocha diffusion is a unique pottery design technique which involves chemical interactions between substances based on particle size, acidity, composition, gravity, and viscosity. The experimental design seeks to find an ideal combination of clay and dendritic slip in which a dendritic arrangement pattern is prominent. A liquid clay slip (primarily alkaline) is treated with an oxide suspension (often acidic) and a dendritic pattern is produced. The experiments focus on utilizing household potter-available chemicals (such as apple cider vinegar, ethanol, water, soap, and lemon juice) for creation of oxide suspension mixtures. The drops of pigments are gathered from chemicals such as iron oxide black, rutile, cooper red, cobalt oxide, titanium oxide and others. Clay slip is poured over a leather-hard dry test tile, and the acid-color mixture slip is used dropwise on top to produce the design. After the formation of a pattern, the test tile is fired in a kiln, leading to a result which may considerably vary from the unfired arrangement. The temperature and the firing can cause the pattern to fade, so concentration of pigment can carry out a crucial role in whether a design is preserved.

Schools of thought are undecided on the exact mechanism of dendrite formation, however, the Marangoni effect combined with concentration diffusion gradients between the slip and the oxide suspension are possible proposed mechanisms. The Marangoni effect is a disturbance in mass transfer within a liquid-liquid medium due to a liquid-liquid interfacial tension. It is observed through the formation of surface tension instability in the region where two liquids interact. In this case, such effect would occur between the liquid acid-oxide suspension and the liquid clay slip.

## Synthesis of Star Polymers via Non-Sugar Alcohols

Daniel M. Goldman

The method of Abiko, Yano and Iguchi was used to explore the application of star polymer branching with cyclic sugars and multi hydroxy aromatic compounds as the core center.

Phloroglucinol, D-Glucose and D-Lactose were reacted with glutaric anhydride via a ring opening reaction to form the individual star-shaped polymer with carboxylic acid terminal groups.

The number of polymer arms formed depended on the reaction conditions as well as the size and the chemistry of the core molecule. Purification of the material by extraction and chromatographic techniques was pursued.

## Formulation and Evaluation of Antibiotic microspheres against Gram-negative *Escherichia coli* and Gram-positive *Staphylococcus aureus*

Miguel Medico <sup>a</sup>, Ayuni Yussof <sup>b</sup>, Dr. Tinchun Chu <sup>b</sup>, Dr. James E Hanson <sup>a,\*</sup>

<sup>a</sup> Department of Chemistry and Biochemistry, Seton Hall University, USA

<sup>b</sup> Department of Biological Sciences, Seton Hall University, USA

Plant-derived flavonoids are a large group of naturally occurring phenylchromones found in fruits, vegetables, tea, and wine. Flavonoids have shown to have a wide range of biological activities, including antiallergic, antibacterial, antiinflammatory, antimutagenic, antioxidant, antiproliferative, antithrombotic, antiviral, and hepatoprotective effects. A certain flavonol glycoside has antiplatelet, antiviral, antihypertensive properties, as well as strengthen the capillaries of blood vessels. These properties are potentially beneficial in preventing diseases and protecting the stability of the genome. Erythromycin (ERY) is a bacteriostatic macrolide antibiotic. ERY is effective against skin and the upper respiratory tract infections caused by Gram-positive bacteria. Poly (DL-lactide-co-glycolide) (PLGA) has been approved for several biomedical applications in humans and is widely used for drug delivery. PLGA has been successful as a biodegradable polymer because it undergoes hydrolysis in the body to produce the original monomers, lactic acid and glycolic acid, which are metabolized in the Krebs cycle to produce carbon dioxide and water. In this investigation, the antibacterial and biological properties of flavonoid-PLGA and erythromycin-PLGA microparticles were studied. Two types of bacterial strains, *Staphylococcus aureus* and *Escherichia Coli* were chosen to evaluate the antibacterial activity of microparticles formed by solvent evaporation technique.

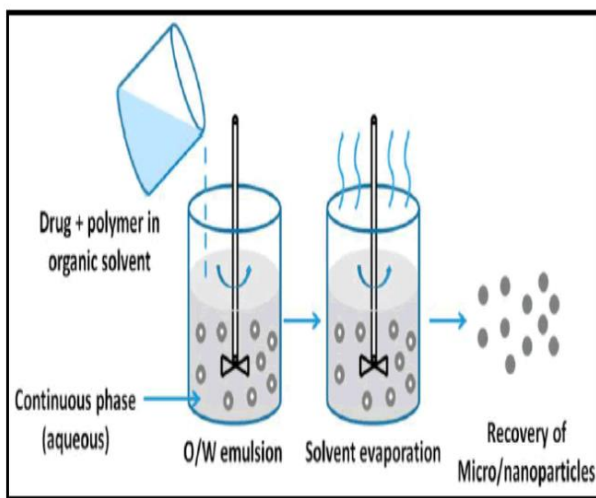
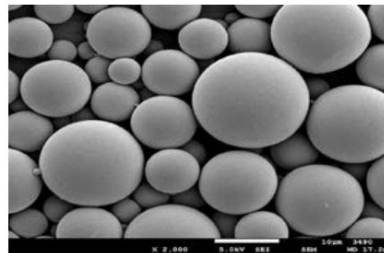


Figure 1: Solvent evaporation technique.



## **The Influence of Pressure and Frictional Heating Influencing Retention in Reversed-phase Chromatography**

Timothy Nowak, Alexey Makarov, and Yuri Kazakevich  
Department of Chemistry and Biochemistry  
Seton Hall University

The usage of sub-2-micron particles in liquid chromatography is very popular in liquid chromatography since faster and more efficient chromatographic separations can be achieved in comparison to traditional (3 $\mu$ m, 5 $\mu$ m) particle size stationary phases. However, the reduction of the particle size leads to a significant increase in backpressure. In addition, heat is generated when the mobile phase passes through a column of finely packed particles. As the heat dissipates through the column, non-uniform temperature gradients can occur both along (longitudinal gradients) and across (radial gradients) the column. However, the environment surrounding the stationary phase bed influences the gradient temperature dissipation. The impact from both the increased backpressure and increased temperature caused by the frictional heating both influence the retention of the analyte. In this study, we study retention behavior of different analytes varying in molecular weight as both backpressure and flow rates are modified.

<b>Title</b>	Indexation of Mixed Mode Adsorbents Using Low Temperature Nitrogen Adsorption and Silica-C18 Surface Energy Scale
<b>Authors</b>	<u>Dinah Lee</u> , Yuri V. Kazakevich

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

## Abstract

Mixed-mode chromatography is becoming increasingly popular in pharmaceutical and biopharmaceutical applications due to its unique selectivity and retention of a variety of compounds [1]. Mixed-mode chromatography is a chromatographic method in which solutes interact with stationary phase through more than one interaction mode or mechanism. It is because of these complex interactions, however, that it is difficult to predict chromatographic behavior of analytes on mixed-mode columns. Characterization of different mixed-mode columns on the basis of surface energy characteristics has not been explored.

The most universal energetic characterization for highly different surfaces could arguably be the C-constant of the BET equation. According to Gregg and Sing [2] C-constant represents the exponent of the excessive energy of nitrogen over its condensation energy at 77 K. In this study, different ratios of porous silica (Luna 5  $\mu\text{m}$  Silica - Phenomenex), and C18 (Luna 5  $\mu\text{m}$  C18 – Phenomenex), single mode adsorbents were blended in various ratios and analyzed by Low Temperature Nitrogen Adsorption (LTNA). A variety of commercially available mixed mode columns were also unpacked and the materials were analyzed by LTNA. Adsorption isotherms, surface area, and BET constants were obtained for all the blended materials in various ratios and the mixed-mode materials.

A linear relationship between the BET C-constant and the blend ratio of silica has been observed. The results from the commercial mixed mode packing material showed similar surface energy characteristics to single mode C18 materials. This data suggests that the BET C-constant maybe a viable parameter that can be used to characterize mixed-mode columns on the basis of surface energy. Utilizing this surface energy scale in conjunction with the study of retention behaviors on mixed-mode material could lead to improvements in the understanding of method development on mixed-mode columns, allow the comparison of commercialized mixed-mode columns, and even predict retention behavior of an analyte in mixed-mode columns.

### Reference:

1. K. Zhang, X. Liu. J. Pharmaceutical and Biomedical Analysis. 128 (2016) 73-88.
2. S.J.Gregg, K.S.W. Sing, Adsorption, Surface Area and Porosity, AP, London, 1982.

**Evaluation of Classical Forcefield Models  
for Multiple Phase Metal Oxides:  $\text{ZrO}_2$ ,  $\text{Y}_2\text{O}_3$ ,  $\text{HfO}_2$**

Jacob Gartlgruber, Tom Melfi, Anastasis Rubino, Maximilian Krejpowicz, and Stephen Kelty  
Center for Computational Research  
Department of Chemistry and Biochemistry  
Seton Hall University

The development of metal oxide device materials ranging from solid oxide fuel cells, sensors and ferroelectrics requires specific crystal phases to be stabilized at the operating temperature of the device. In many cases, the optimal phase is thermodynamically unstable relative to other phases. A common practice is to dope guest atoms into metal oxides to provide greater stability of the desired phase. Common examples include the cubic phase of  $\text{ZrO}_2$  and  $\text{HfO}_2$  doped with yttrium atoms which are frequently used to SOFCs and ferroelectrics, respectively. This study is aimed at using atomistic modeling to investigate the structural properties of doped metal oxides that lead to the desired ferroelectric response of these materials. An essential aspect of the study is to develop and validate reliable models that will allow valuable prediction of these properties. Due to the large system size ( $10^3$  –  $10^5$  atoms) to be investigated, classical models are preferred. Several models have been published but require validation over several crystal phases of each material. Often, classical forcefields are developed which, while being well suited for a particular crystal phase, are not capable of modeling the several phases that may be present in laboratory-prepared materials. We provide a survey of published forcefield's ability to adequately model several likely crystal phases to allow for selection of optimal classical models for future work.



**Title**

Development and optimization of a pair of experiments for the teaching laboratory based on the synthesis of biodiesel

**Authors**

Milind Das, Jaiveer Gill, Gauri Patel, Ronit Paul, Ariana Shatynski, Shubham Singh, and David A. Laviska

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

**Abstract - 300 words maximum**

As global reliance on fossil fuels becomes increasingly fraught with questions related to issues involving ethics, equity, economics, politics, and sustainability, renewable sources of energy are receiving more attention than ever before. Financial and infrastructural investments in the development of solar and wind power, hybrid/electric modes of transportation, and renewable sources of molecules suitable for combustion are growing rapidly. As one example, “biodiesel” is fast becoming part of our vernacular (at least in the U.S.), even if few consumers know much about it – what it is, where it comes from, why it has the prefix “bio”. As one initiative under the umbrella of the newly christened Academy for Green Chemistry, Stewardship, and Sustainability at Seton Hall University, we are developing experimental protocols for our teaching laboratories that involve a systems thinking approach to the fundamental chemical concepts that we hope will resonate with students far beyond the doors of the classroom. One of the prime focuses of our research group involves piloting and optimizing these protocols to be certain they adhere as much as possible to the tenets of green chemistry while also teaching chemical concepts and inspiring students to think about broader issues such as sustainability and stewardship of the planet. In this poster, we will describe a simple, inexpensive, highly reproducible synthesis of biodiesel. We will also outline the aspects of the protocol that are especially “green” as well as discuss why/how this protocol can be tailored to serve students in either general chemistry or organic chemistry courses.

**Title**

Developing greener syntheses of polyaromatic ligands and novel late transition metal complexes

**Authors**

David Essien, Kareem Fakry, Rhys Vaughan, and David A. Laviska

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

**Abstract - 300 words maximum**

The tenets of Green Chemistry are infused throughout all research projects in our group, including the synthesis of bi-, tri-, and polyaromatic molecules for use as multidentate ligands in transition metal complexes. Having successfully synthesized a large family of ligands based on a quinoxaline skeleton (previously reported), we are working to broaden the scope of these reactions and use them as a starting point for developing new synthetic routes to more elaborate molecules that may be good candidates for both cyclometalating and/or bridging ligands. We anticipate that these ligands may impart desirable photophysical properties and/or chemical reactivity when coordinated to metals. To date, we have synthesized substituted pyrazines, quinoxalines, and benzoquinoxalines, and have completed some preliminary studies of their metal complexation reactions, all utilizing methods with enhanced adherence to the tenets of Green Chemistry. In this poster, we will present details of the syntheses, greener aspects of the reactions, and characterization of products.

**Title**

Greener synthesis and characterization of a family of bidentate quinoxaline-type ligands and their use in several late transition metal complexes

**Authors**

Anthony Rodriguez and David A. Laviska

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

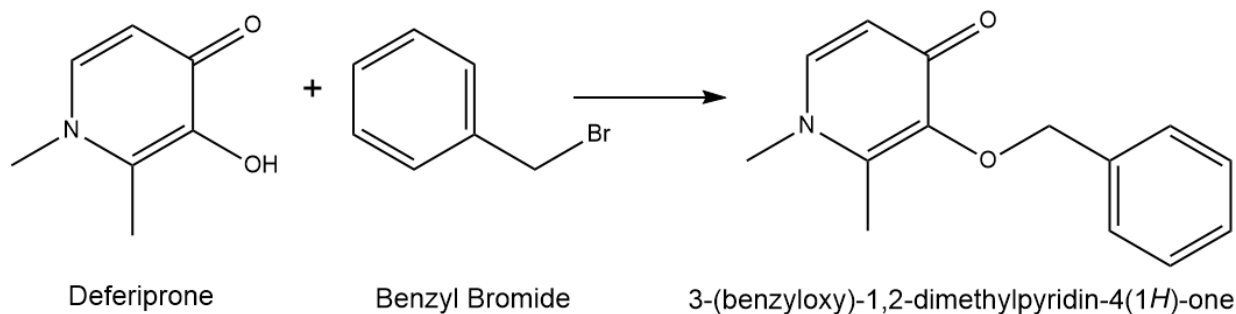
**Abstract - 300 words maximum**

Polyaromatic molecules are commonly used as multidentate ligands in transition metal complexes due to their highly tunable steric and electronic properties as well as metal-coordination modes. Quinoxalines, or benzopyrazines, are a class of heterocyclic aromatic compounds that haven't found wide industrial relevance beyond use as components of certain dyes or as parts of larger molecules with pharmaceutical relevance. However, with strategically chosen substituents, the quinoxalines can be useful ligands in transition metal complexes that exhibit unique photophysical properties. In order to investigate the physical and chemical properties of complexes containing these ligands, we have synthesized a series of substituted quinoxalines using newly developed protocols that are significantly greener than literature precedents. To date, we have synthesized and fully characterized twelve quinoxaline-type ligands in good-to-excellent yield and high purity using these protocols. These ligands fall into three general classifications: diphenyl, difuranyl-, and dipyridylquinoxalines. In this poster, I will present the synthetic strategies we have used as well as results and characterization of both ligands and metal complexes.

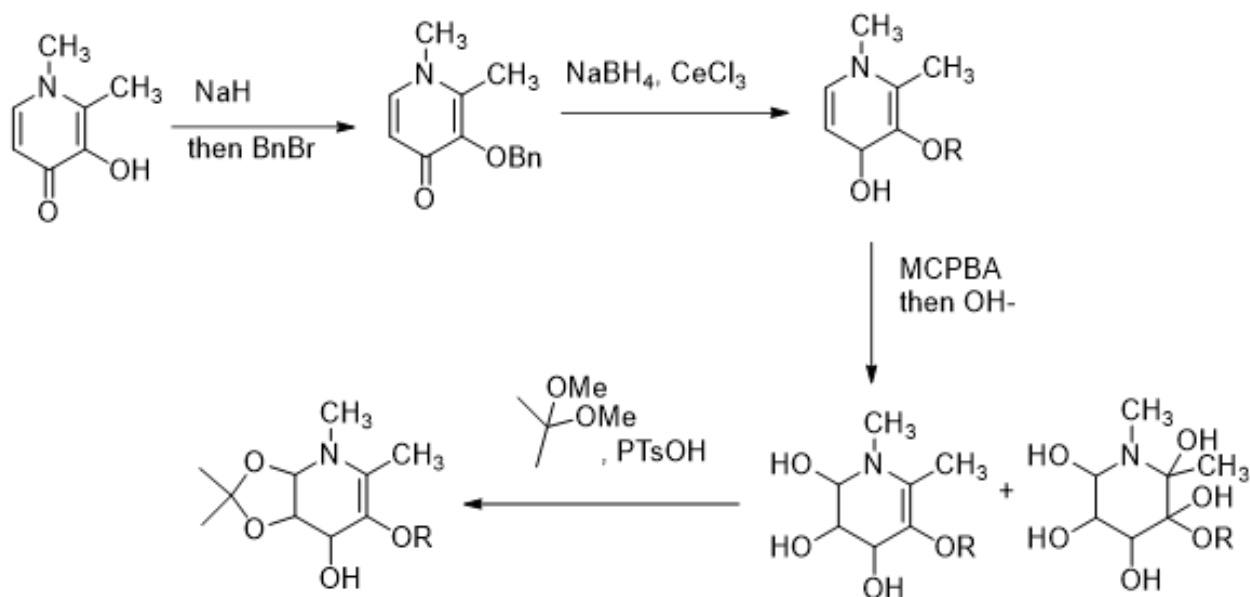
# The Synthesis of a Potential New Epilepsy Drug

Giannini, Leonarda; Roundy, Dean; Marzabadi, Cecilia

In this project, studies have been done on a compound Deferiprone (3-hydroxy-1,2-dimethylpyridin-4-one) which is currently being used as an iron chelating agent in treating iron overload. The goal of the project is to a Nitrogen analogue of a hexose sugar, and to yield a compound that could potentially be effective in epilepsy treatment. Thus far, is the protection of the Hydroxide group on the molecule of Deferiprone has been carried out with Benzyl Bromide since the OH group is very reactive.



Next, we will selectively reduce the ketone moiety, using a Luche reduction. Then the double bonds will be dehydroxylated. Finally, one of the vicinal diols will be protected as an acetal. The final product will be submitted for testing.



## **Povarov Cycloaddition of Cyclic vinyl ethers with Phenyl-(1-phenylethylidene) amine**

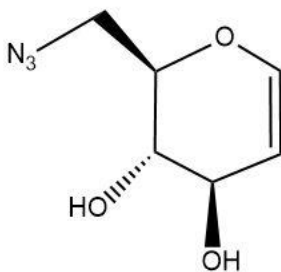
John Michael Benedict B. Unciano and Dr. Cecilia Marzabadi

In this project, we investigated the Povarov cycloaddition reaction Tri-O-Benzyl-D-Glucal and Phenyl-(1-phenylethylidene) amine to synthesize a quinoline as a potential anti-cancer drug. Previously, we had synthesized quinolines using the imine of an aldehyde and we wanted to investigate the products formed from the imine of a ketone. Both conventional and microwave studies were carried out. However, H-NMR and mass spectrometry results suggest that the desired compound was not to formed and this may be due to the steric hindrance from Tri-O-Benzyl-D-Glucal. The studies were repeated using the less sterically hindered Dihydropyran. The results of these studies will be reported.

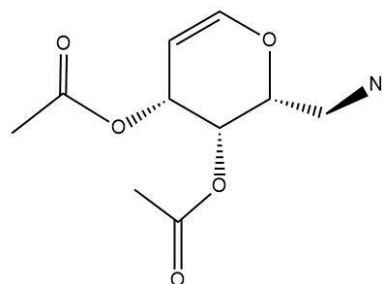
### Novel Carbohydrate Analog Synthesis for Potential Contribution to CNS Disorder Treatment

Central Nervous System (CNS) disorders are a prevalent and devastating class of illnesses. One of the major challenges for creating drugs that address CNS disorders is the blood-brain barrier as many molecules cannot cross through into the brain due to tight junctions between endothelial cells. Therefore, carbohydrate analogs can be employed to help in the treatment of CNS disorders because they have high biocompatibility and can be easily modified for certain receptor proteins since sugars can cross the blood-brain barrier through glucose transporters (GLUT). Two different approaches were used to synthesize an azide-containing carbohydrate, both utilizing an intermediate molecule with a tosylate side chain. In method one, tri-hydroxy-glucal was used as the starting material, while the second method used D-galactal as the starting material. The structure of the desired product for each approach is shown below. Ultimately, the azide group will be reduced to form the amino sugar, and then cyclized to give an oxazoline. Further studies can potentially involve synthesizing different analogs and examining the effectiveness of the molecules in CNS disorder treatments.

Method 1



Method 2



**Title:** Microwave synthesis and photophysical characterization of novel heteroleptic iridium complexes containing polyaromatic C<sup>^</sup>N and N<sup>^</sup>N ligands

**Authors:** Allyson D. Dixon, Wyatt R. Murphy.

Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079

**Abstract:** Organic Light-Emitting Diodes (OLEDs) and Light Emitting Electrochemical Cells (LECs) are of increasing interest due to their ability to serve as alternative light sources. The main emissive components of these devices are typically ionic transition metal complexes (iTMCs). Iridium (III) complexes are of particular interest due to their desirable photophysical properties such as high radiative quantum yields, relatively short excited-state lifetimes, and overall stability. As such, the potential for their use in OLEDs/LECs and as photodynamic therapy (PDT) agents has inspired vigorous research into the improvement and/or modification of existing protocols for the preparation of the iridium (III) complexes themselves. A common challenge in the class of reactions is the requirement for long reaction times (often greater than 24 hours reflux) followed by extensive isolation and purification steps. We have utilized a microwave reactor to bring our research into closer alignment with the tenets of green chemistry. As an extension of this effort, we have synthesized a library of heteroleptic, cationic iridium (III) transition metal complexes (Ir-iTMCs) using microwave heating, resulting in drastically reduced preparation times compared with conventional heating, increased purity, and percent yield as reported in the literature. Beginning with compounds of the general formula  $[\text{Ir}(\text{pq})_2(\text{N},\text{N})]^+$  (pq = 2-phenylquinoline; N,N = cuproines), we have expanded the ligand scope and synthesized a range of novel complexes. We will discuss both the procedural details of our versatile synthetic protocol as well as the characterization and photophysical properties of selected complexes.

Roksana Najar, Jose Ruiz-Perez, & Joseph A Gil

Petersheim Abstract

29 March 2022

Department of Chemistry and Biochemistry

Optimization of the Green Synthesis of Cyclometalated Complexes of Iridium(III) with Methyl Phenantrolines

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). Our work will build upon our previous work in which Ir-iTMCs containing neocuproine and bathocuproine respectively, were synthesized. Specifically, we will be strictly focusing upon a variation of dative ligands to improve our current synthetic methods and assess the impact of simple structural features on the photochemical properties. The three dative (N<sup>^</sup>N) ligands that are going to be studied are 1,10-phenanthroline (phen), 4-methyl-1,10-phenanthroline (4-Me-phen), and 5-methyl-1,10-phenanthroline (5-Me-phen). The importance of functionalization of ligands can be explained by the nature in which overall electronic properties are manipulated to produce a range of color. The goal of this project will be updating the current and earlier synthetic methodologies to be green, high yield, fast with minimal purification, and improve the cost of manufacturing to increase the quality of OLED and LEC screens.



**Title**

Optimization of Microwave Synthetic Conditions for [Ir(ppy)<sub>2</sub>(2,2'-bipyrimidine)](PF<sub>6</sub>) and [Ir(ppy)<sub>2</sub>(2,2'-bipyridine)](PF<sub>6</sub>) (ppy = 2-phenylpyridine).

**Authors**

Nataly A. Areosa Suarez, Florian Balan, Daniela Moncada, Allyson Dixon and Wyatt R. Murphy, Jr.

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**Abstract - 300 words maximum**

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.

Since the original discovery of this unique bifunctional interaction, a rich chemistry of homo- and heteroleptic complexes of Ir(III) with cyclometallating ligands such as 2-phenylpyridine involving simultaneous metal-nitrogen and metal-carbon bonds has advanced. These reactions require reflux times of 18 to 24 hours, which impedes rapid progress. A developing area of chemistry involves the use of commercial microwave chemical reactors to conduct the reactions in significantly shorter periods while minimizing environmental damage. <sup>(3-5)</sup> The Department of Chemistry and Biochemistry is also incorporating green chemistry principles into the curriculum. In accordance with this goal, an evaluation of microwave reactors from several manufacturers was made by the Murphy research group, along with developing new microwave-based reaction conditions. With two years of trials completed, further analyses are being made to evaluate the efficiency of the group results.

The group is currently looking into [Ir(ppy)<sub>2</sub>(2,2'-bipyrimidine)](PF<sub>6</sub>) and [Ir(ppy)<sub>2</sub>(2,2'-bipyridine)](PF<sub>6</sub>). After, establishing a concrete procedure using the microwave, and producing a sufficient amount of these products, further examinations were conducted including quantum yield, NMR, and lifetime.

<b>Title</b>	Synthesis and characterization of biodiesel using microalgae as sustainable triglycerides source
<b>Authors</b>	Staes*, Goncalves, Tate, Mitchell, Mathews, Murphy

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

## **Abstract**

Biodiesel is diesel fuel produced from vegetable oils, mainly consisting of a mix of Fatty Acid Methyl Esters (FAME) that are obtained through the transesterification of these vegetable oils with an alcohol. This research project focusses on synthesizing biodiesel fuel from microalgae because of their unique advantages as triglyceride source. Their fast growth, high lipid content, and essential role in the global carbon cycle due to their ability to perform photosynthesis make them a promising biofuel triglyceride source. Algal growth was monitored by taking the absorbance at 600 nm using UV-Vis spectroscopy and allowed for optimization of algae yield and identification of ideal algae species. The microwave-assisted oil extraction method and transesterification reaction were based on selected research experiments from literary sources, allowing the synthesis of biodiesel to be intensively studied with the goal of optimizing this process. The biodiesel produced will be analyzed by gas chromatic methods. Further studies on biodiesel production and alternative fuel sources will encourage the large-scale production of biofuels and will aid in the global transition to more sustainable and environment-friendly energy sources.

**Title**

Extraction, Qualitative and Quantitative Analysis of Clove Oil using Gas Chromatography

**Authors**

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**Abstract - 300 words maximum**

Gas chromatography is a method of separation in which substances are passed through a stationary and mobile phase to distinguish its components. When used in conjunction with mass spectrometry, these components become easily identifiable. Gas chromatography, specifically, uses helium gas as the mobile phase to carry the compounds of interest through a column. As each compound is moved through the column, it interacts with the stationary phase, which can be either polar or nonpolar. These interactions are represented graphically as peaks on a 2-dimensional graph, and compounds can be identified by their polarity.

In this research, a Lucidity miniature gas chromatograph and a standard Shimadzu gas chromatograph were used to analyze samples of clove oil. Clove oil is recognized for its variety of medical applications, especially in topical pain relief and cavity prevention, as well as use in cosmetics and antibacterial agents. Using Gas Chromatography, separation of the components of clove oil were performed. This qualitative data was then used to compare the methods of chromatography in their ability to separate and distinguish compounds from clove oil. The chemical makeup of the clove oil was analyzed using this data. Clove oil was extracted from dried cloves using the methods of steam distillation and microwave-assisted extraction. The oils obtained by these processes were analyzed by gas chromatography and their components will be compared to store-bought clove essential oil.

**Title**

Comprehensive Two-dimensional Gas Chromatography-Time of Flight Mass Spectrometry of Pesticides

**Authors**

James D. Mizvesky and Nicholas H. Snow

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**Abstract - 300 words maximum**

Society has seen an increased interest in health and avoiding consumption/exposure to toxic chemicals, such as pesticides, as seen by the increase in products deemed "organic and natural". Pesticides are any substance used to kill, repel, or control certain forms of plant or animal life that are considered to be pests, containing both "active" and "inert" ingredients, as defined by the NIH and EPA. Governments around the world have even acted through rules and regulations to protect its citizens and environmental lands from consumption/exposure. These rules and regulations are greatly slanted towards preventing consumption for obvious reasons, but arguably little to no attention is placed on exposure through other commercially available products, such as cut flowers to even aromatic oils and perfumes. The cut floral industry is one of the sectors where regulation is not necessarily protecting the consumer but are geared towards the prevention of pest traveling from on area of the world, typically Colombia and Ecuador, to the USA. Typically, pesticides are identified through using various chromatographic methods such as GC-MS and LC-MS. Although their metabolites tend to be the ones identified due to a variety of factors, such as degradation over time, time of sampling, and sampling method. This work uses Two-dimensional Gas Chromatography-Time of Flight Mass Spectrometry (GCxGC-ToFMS) enhanced sensitivity to identify and characterize pesticides, typically used in the cut flower industry. The lower Limit of Detection provided by the GCxGC-ToFMS will allow for easier identification of pesticides, provide crucial information about pesticide application cycles and when/if exposure levels are of concern.

**Title**

Analysis of Lavender Essential Oil and Valerian Root by Gas Chromatography and Microwave Extraction

**Authors**

**Bitha Beji and Nicholas H. Snow**

*Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079*

**Abstract - 300 words maximum**

Gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS) are an integral part of the science and technology field regarding the analytical processes of various compounds. While the gas chromatograph vaporizes a sample into the gas phase and separates its components at the liquid phase, the mass spectrometer ionizes these components and identifies them using their respective mass-to-charge ratios. These instruments have been vastly utilized in the detection of drugs, environmental studies, and the identification of unknown samples, which will be its primary application in this research.

Lavender, also known as *lavandula*, is a culinary herb that has been known to have many health benefits, such as the reduction of blood pressure and heart rate, and relief of asthmatic symptom and inflammation. It may also offer a natural remedy for pain, and it has aromatherapy applications as well. Most importantly, for purposes of this research, it has been shown to induce sleep. Through other studies, it was determined that linalyl acetate, linalool, camphor, and lavandulol are the main chemicals within lavender that produce this sedative effect, due to their rapid absorption into the bloodstream. In order to further analyze these compounds and their properties, Lucidity miniGC, Shimadzu Nexus GC-2030, and Hewlett Packard GC-MS will be used to separate and identify the various components of commercially available lavender essential oil. In addition, commercially available valerian root, or *valariana wallichii*, will be examined, as it has similar sedative properties as lavender. The effects of different instrumental and extraction techniques will be studied as well, such as microwave extraction and steam distillation, as it relates to green chemistry. The advancements with this research can be used to better understand these sleep-inducing compounds in order to aid insomnia and observe its effects on the brain.

## **COMPARATIVE STUDY OF CHROMATOGRAPHY SIMULATION MODELS AND THEIR IMPORTANCE IN GC ANALYSIS**

Nicole K. Charles and Nicholas H. Snow  
Department of Chemistry and Biochemistry (Seton Hall University)

Chromatographic separation processes represent the method of choice for the purification of species characterized by low selectivity, especially useful drug development. At the same time, the need for effective modeling methods to study these processes has emerged since the inception of research in separation sciences and various modeling schemes have been proposed with different degrees of complexity. As a result, chromatography simulation models present various capabilities, such as modeling the effects of pressure programming, column dimensional changes, serially coupled columns, and peak broadening. Optimization of these models mostly aims at improving the process performance based on the current modelling and providing general guideline or trends for the separation systems.

The main goal of this study is to present a thorough review of previous chromatography models and demonstrate how they compare with newer simulation program compares with other commercially available HPLC and GC simulations programs in particular EZGC, DryLab and developed in-house software. We also compare the separation performance through our simulation and optimization in other to better understand why a given operational mode performs better or worse than other readily available chromatography programs. In this manner, the proposed methodology could provide some complete insights into some principal mechanisms of separation techniques. Comparison is established between obtained results and outputs from readily available programs such as Restek EZGC simulation software and more as a way to better understand elution models and to predict chromatographic retention times which can influence overall analytes separation.



**Title**

Development of various gas chromatography methods to detect analogs of fentanyl

**Authors**

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**Abstract - 300 words maximum**

Fentanyl, originally designed for use as a narcotic analgesic in clinical settings, has recently become a new focus in the field of forensic casework and drug related investigations. This substance has proven to be a considerable challenge to be analyzed in the field due to the quantity of fentalogs that exist of the substance—edited versions of the opiate with different functional groups that have evolved faster than the technology used to detect them. This study aims to develop new gas-chromatography standards in the field of forensics that focus on the detection of fentalogs with different functional groups, such as those which involve different gas eluents or solid-phase microextraction. These different methods and other similar novel approaches to efficient, time-sensitive detection of narcotics will prove essential to forensic analysis as the issue of opiate use progresses.

**Title**

Re-examination of Gas Hold-up Time in Gas Chromatography

**Authors**

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**Abstract - 300 words maximum**

In gas chromatography, the gas hold-up time ( $t_m$ ) is the time required for an unretained compound to elute from the column. It is a function of several physical parameters: carrier gas viscosity ( $\eta$ ), the column dimensions (L and r), the inlet and outlet pressures ( $P_i$ ,  $P_o$ ) and their ratio (P). Over the temperature range in GC, the exponential relationship between gas viscosity and temperature approximates as linear (at constant pressure), so if the retention time of a substance increases linearly with temperature, then the substance is unretained, and can be used for gas hold-up time measurement. This relationship has been utilized within this research to present other compounds to deduce gas hold-up time. Other compounds are needed since the commonly used ones nowadays – methane and butane, cannot be injected without removing the attached autosampler present on almost all gas chromatographs. Thus, research was done into the effectiveness of the injection of other pure compounds to deduce an accurate hold-up time value. Furthermore, an overall presentation of different methods for gas hold-up time acquisition throughout the literature is presented in order to re-examine it for a clearer picture, as well as for comparative value. Lastly, the accuracy of the hold-up time value was examined with respect to multiple variables affecting the value, including column length, diameter, a flow rate. Multiple compounds on multiple columns were found to be suitable for  $t_m$  measurement, and the analysis of the literature allowed the new data to be shown in a broader scope.



**Title**

Polyol-induced Extraction and UHPLC-MS/MS for the determination of NSAIDs in water and urine

**Authors**

Shipra Patel and Nicholas H Snow

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**Abstract - 300 words maximum**

Polyol-induced Extraction is used for the extraction and analysis of NSAIDs. This is an expansion of our initial project of evaluating PIE as an extraction method. Polyol-induced extraction is an extraction technique developed and patented by Drs. John Sowa, Wyatt Murphy, and Mithilesh Deshpande at Seton Hall University, as a technique for removing water from mixtures with polar organic liquids. In Polyol-induced extraction, a solvent mixture of acetonitrile and water can be separated by adding a polyol mass separating agent such as glycerol, sorbitol, erythritol, xylitol etc. The focus of this work is to demonstrate polyol-induced extraction as an effective extraction technique in trace analysis of drugs. In this work Glycerol is used as a mass separating agent in the extraction of NSAIDs from water into polar organic solvents. Eight different NSAIDs were extracted by polyol-induced extraction and were analyzed by UHPLC-MS/MS. MRM transitions were evaluated for each compound for the identification and quantification. Percent recovery and partition coefficients, accuracy, precision, limit of detection and limit of quantification were determined for each NSAID. The NSAIDs under this study included ibuprofen, indomethacin, aceclofenac, tolafenamic acid, ketoprofen, naproxen, mefenamic acid and, oxaprozin. NSAIDs extraction was performed in 1:1 ACN/Water mixture using Glycerol. Upon analysis of these drugs in water extraction of these drugs was performed from a synthetic urine sample to evaluate PIE as an extraction method.

**Title**

Qualitative Analysis of Biodiesel Fuel Samples Derived from Algae Using Gas Chromatography and Mass Spectrometry

**Authors**

Ria Sandeep, Nicholas H. Snow, Wyatt Murphy

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**Abstract**

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.

## Investigating the interaction of azobenzene moiety on nearby amino acids

### Abstract

Molecular photoswitches are a series of compounds that can be isomerized upon irradiation with light. They are used to control protein structure and function with temporal and spatial precision. Azobenzenes are a family of compounds that can undergo a reversible *cis-trans* photochemical isomerization. Irradiation around 330 nm converts the thermodynamically stable *trans*-isomer azobenzene compound to the *cis* isomer, while the *cis* form reverts thermally upon irradiation at 420 nm or higher wavelengths. The two isomers differ in geometry and dipole moment. As a result, the placement of an azobenzene moiety near a substrate or ligand binding site in an enzyme, receptor, or ion channel allows the reversible modulation of the binding affinity and the activity of a protein. However, more research is needed to be known about the mechanism or the effect of the azobenzene moiety on nearby amino acids. My work is a preliminary investigation of the possible interaction between azobenzene and aromatic amino acids.

**Title**

Illuminating Membrane Active Peptides

**Authors**

Cristina Ventura, Gregory Wiedman

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**Abstract**

Many  $\alpha$ -helical membrane active peptides (MAPs) contain a central proline residue that creates a kink in the helix. The helix-disrupting nature of proline can be mimicked by azobenzene, a photoisomerizable molecule. Azobenzene can be converted from its *trans* to *cis* isomer by excitation with ultra-violet light and from its *cis* to *trans* isomer by excitation with visible light. In this work proline containing membrane active peptides are studied by substituting proline for azobenzene on the backbone of the MAP. The photostationary state of the *trans* and *cis* isomers of the photo-peptides is sequence dependent. These peptides retain the secondary structure of the native peptides while exhibiting light dependent activity.

# Inhibiting infectivity of murine hepatitis virus A59 (MHV-A59) by targeting peptide organometallic compound to spike protein

Makayla Manfredi, Dr. Gregory Wiedman, Dr. Daniel Nichols, Dr. Wyatt Murphy

Department of Chemistry and Biochemistry, Seton Hall University, South Orange NJ 07079

## Abstract

Murine hepatitis virus A59 (MHV-A59) is a coronavirus that infects mice with diseases similar to human conditions. Pseudoviruses are useful to determine mechanisms of action in viral infectivity because of their versatility and safety. 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. The S protein on viruses is responsible for membrane fusion and mediating receptor binding. The development of peptides analogous to regions outside the fusion spike protein are the basis for inhibition of viral infectivity. In recent studies, the combination of specified peptides and photosensitizers have demonstrated promising results regarding treatment of infections through photodynamic techniques. 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 oxygen to initiate cell death. This presentation discusses the development of a targeting peptide attached to a photosensitizer organometallic complex in order to inhibit and kill virus particles through its spike protein.

Key words: pseudovirus, spike protein, peptide, photosensitizer, photodynamic therapy

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**Title**

Photosensitizer-membrane-active peptide conjugates for *C. auris* inhibition

**Authors**

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**Abstract**

*Candida auris*, an opportunistic fungus responsible for causing candidemia and candidiasis in immunocompromised individuals, has been a recent topic of interest for infectious disease researchers. Since its isolation from a patient at Tokyo Metropolitan Geriatric Hospital in 2009, *C. auris* has been identified in four separate geographic regions: South Asia, East Asia, South Africa, and South America. Phylogenetic analysis of clinical isolates from each of these regions reveals a lack in genome consensus, indicating that *C. auris* arose independently. As such, *C. auris* strains are classified as members of a clade, or a group sharing a common ancestor. Due to its ability to survive under stressful conditions, such as elevated temperatures and increased salt concentrations, there is speculation that the emergence of this species is related to increasing global temperatures.

Despite rising concerns over multidrug resistance (MDR) in microbial pathogens, the development of clinically approved antifungal treatments has remained stagnant in recent decades. Apart from ibrexafungerp, a newly approved triterpenoid glucan synthase inhibitor, most *Candida*-related infections have been treated with polyenes, azoles, and echinocandins. *C. auris*, in particular, has displayed MDR to these antifungal agents. The most often observed resistance mechanisms are mutations to drug targets and upregulation of efflux pumps.

In order to circumvent these resistance pathways, we propose a dual-functioning photosensitizer-peptide conjugate for the inhibition of *C. auris* growth. Photodynamic therapy (PDT)<sup>4</sup>, used for decades to treat a wide range of illnesses, has antimicrobial applications. Combined with a membrane-active peptide, the photosensitizing agent can localize within target cells and generate singlet oxygen. Ir(ppy)<sub>2</sub>dicarboxy(bpy)<sub>2</sub> was coupled to the peptide portion of the conjugate using an Fmoc-based synthetic strategy and tested against *C. auris* strains in vivo.

**Title**

Continued investigations into a Cryptococcal Antifungal Peptide

**Authors**

Robert J. Tancer, Gregory Wiedman

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**Abstract**

To expand on the work presented at the Petersheim symposium last year (2021), the author sought to rationalize the activity of the Cryptococcal antifungal peptide dubbed AW9-Ma. This peptide is a potent flippase inhibitor that leads to significant accumulation of phosphatidylserine (PS) on the outer membrane leaflet of the cell as well as growth inhibition on its own at 64µg/mL. This peptide potentiates the effects of caspofungin when mixed in a checkerboard assay leading to an FIC index of 0.5. The peptide was also somewhat hemolytic. Protein databank structures of the principle PS flippase in red blood cells, ATP11C-CDC50a were analyzed using pymol software, and a 14Å distance between the binding pocket of PS and the drug analog in CDC50 loop region was found supporting the canonical binding model of flippase activity. Subsequent peptide modifications lead to dramatic improvement of the antifungal activity of the peptide.



**Dr. Matthew Petersheim**  
**1953-1998**