ROSE MERCADANTE SEMINAR SERIES

Department of Chemistry and Biochemistry 26th Departmental Symposium in Conjunction with the Petersheim Academic Exposition

Book of Abstracts

This year's event will take place virtually
https://blogs.shu.edu/symposia/petersheim-2021-chem_bio/
April 27, 2021

Keynote Lecture: 5:45 – 6:45 PM
Johannes Zakrzewski, M.D.
HMH CDI

Poster Session: 7:00 – 9:00 PM

7:00 – 8:00 Poster Authors 1-21 Present
8:00 – 9:00 Poster Authors 22-45 Present

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Keynote Lecture

Targeting NF-kB in B Cell Malignancies

Johannes Zakrzewski, M.D.
Hackensack Meridian Health
Center for Discovery and Innovation

Abstract: Multiple myeloma (MM) is the second most common blood cancer, accounting for almost 32,000 new cases in the US per year. Even though considerable progress has been made over the past decade, and most newly diagnosed patients will survive for more than five years, there is still no cure for MM and all patients eventually become refractory to currently available therapies. It is therefore critically important to develop new drugs and treatment regimens with new mechanisms of action against MM cells. One of the molecular pathways known to promote survival and resistance to chemotherapy of MM cells includes NF-kB, a pathway with important functions in both healthy and diseased cells, including a wide range of cancer cells. We recently developed a direct NF-kB inhibitor reducing DNA binding of all five NF-kB subunits, resulting in potent inhibition of transcriptional activity mediated by both canonical and non-canonical NF-kB pathways. We confirmed that strong anti-myeloma activity of our drug candidate was associated with little signs of toxicity in experiments with MM cell lines, patient-derived MM cells, and mouse models of MM.

Bio: I obtained an MD degree from the Friedrich-Alexander University (Germany) in 2000, followed by 5 years of training in Pediatrics and Pediatric Hematology/Oncology in Germany. I joined Memorial Sloan Kettering Cancer Center (MSKCC) in 2004 as a Research Fellow, studying the immunology of allogeneic hematopoietic stem cell transplantation. From 2008 – 2012 I was a resident in Pediatrics at SUNY Downstate Medical Center and a clinical fellow in Pediatric Hematology/Oncology at MSKCC. From 2012 – 2017 I was an Assistant Attending Physician at MSKCC. In 2018 I joined the HMH CDI as an Associate Member, and I am also an Attending Physician in Pediatric Stem Cell Transplantation at HUMC. I have additional appointments as an Associate Professor at Hackensack Meridian School of Medicine and Georgetown University School of Medicine.

Dr. Cosimo Antonacci

1.

Testing the Glucose Levels of Foods and the Relevance of High Sugar Levels to Public Health

Lachelle S. Dufresne, Cosimo Antonacci*, and Gerald Buonopane *

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

Food insecurity is prevalent among minority women and has severe implications for not only their health but also the health of their children. Food insecurity is defined as "limited or uncertain availability of nutritionally adequate and safe foods or limited or uncertain ability to acquire acceptable foods in a socially acceptable way." Women who are food insecure often are deprived of the needed nutrients (vitamins, calcium, iron, the 8 essential amino acids, 2 essential fatty acids, folic acid, and energy) which often lead to the health issues of their children. It is the nutritional deficiency component that contributes not only to this population of society but has broad public health implications. While necessary vitamins and minerals are absent in the diets of the food insecure, high levels of harmful food additives are extremely prevalent. Particularly, high levels of sugar have been found to affect cognitive development and contribute to metabolic syndrome. The focus of this research project is to educate students on the effects of high sugar levels on one's health while also bringing to light the social implications of this health issue.

2.

Porphyrin Synthesis and Quadruplex Binding

Brennan Isaac, Usha Kalra, Cosimo Antonacci*, and Dr. James E. Hanson*

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Quadruplexes are DNA structures formed from G-rich sequences. Together, they form a tetrad stabilized by non-canonical base pairing. Certain sequences can allow for multiple tetrads to form and stack upon each other. These G-rich sequences have been found in a variety of places in the human genome. By interacting small molecules with these sequences in a structure specific manner, one may be able to modulate the stability of these quadruplexes and potentially any downstream products related to those sequences. Herein, we present progress toward the synthesis of novel porphyrin and related quadruplex binding studies using analytical techniques like UV-VIS, Circular Dichroism, Proton NMR, and Mass spectrometry.

Dr. Joseph Badillo

3.

In Silico Drug Design: Docking of the COX2 Enzyme

Milan Patel, Jennifer Orth, Seung Nam, and Joseph Badillo*

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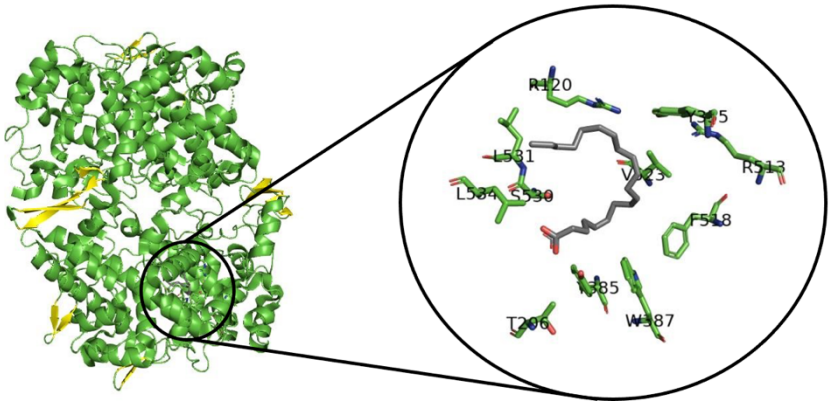

Computational chemistry is a powerful method for understanding how small molecules interact with target enzymes. COX2 is a key enzyme that converts arachidonic acid to prostaglandins, which are responsible for pain and swelling at a wound site. Inhibitors of this enzyme are essential to combat excessive inflammation. Using processes developed by the Tantillo Lab at UC Davis, this presentation will discuss the in silico (computer-based) docking of small molecules into the COX2 active site. A variety of freely available software applications was used to visualize enzyme structure and optimize small molecules to determine binding affinity. This project lays the groundwork for the Badillo Group's ability to visualize any enzyme we choose and formulate drug candidates that have the potential to treat human disease.

4.

Photoredox-Catalyzed Meerwein Arylation of Benzofuran and Benzothiophene

Vanessa Colmenares, Shreya Rawat, Nancy Habib, Pooja Bhate, and Joseph Badillo*

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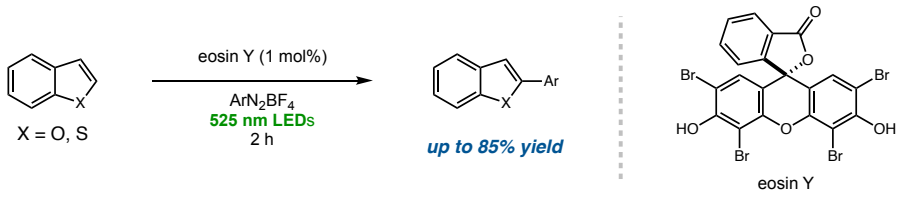

In recent years photoredox catalysis has emerged as a powerful tool for the synthesis of small molecules. The Meerwein arylation is a reaction that involves the coupling of an aryldiazonium with an alkene. This presentation will discuss the development of a photoredox-catalyzed Meerwein-type arylation with benzofuran and benzothiophene and a variety of substituted aryldiazonium salts to from the corresponding 2-arylbenzofurans and 2-arylbenzothiophens. This mild reaction protocol provides an alternative route to current methods enabling access to these important molecular scaffolds used for the synthesis of pharmaceuticals and natural products. The effect of different photocatalysts, solvents, and light sources on reaction efficiency will also be discussed.

5.

Organo-Lewis Photoacid Catalyzed Synthesis of Amines

Andrea Serrano Trujillo and Joseph Badillo*

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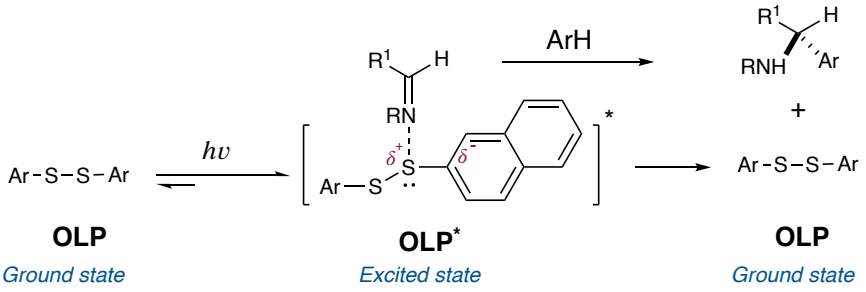

This project focuses on the development of an organo-Lewis photoacid catalyst for the synthesis of an amines from the corresponding imines. Upon irradiation, excited-state disulfide containing aromatics such as 1,2-di(naphthalen-2-yl)disulfane become potent Lewis acids that can be engaged in catalysis.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

6.

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

Jason Saway, Ali Akram, Mackenzie McCann‡, Joshua Novello‡, Suzanne Gantar‡*, and Joseph Badillo*

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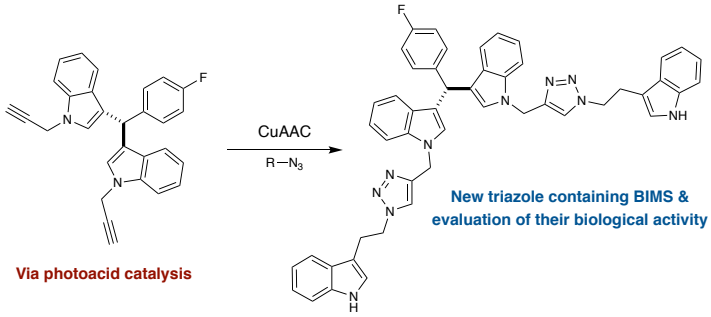

Our laboratory recently developed a mild photoactivated strategy for the synthesis of bis(indolyl)methanes and 3,3'-di(indolyl)oxindoles. Bis(indolyl)methanes (BIMs) are of interest due to their interesting anti-cancer properties. This presentation will discuss the synthesis of a variety of triazole 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.

7.

Photoacid-Catalyzed Acetalization of Carbonyls

Abigail Pierre, Jason Saway, and Joseph Badillo*

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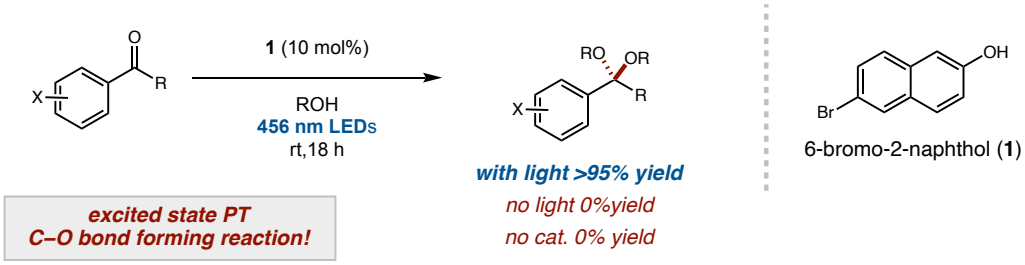

Photoacid-catalyzed processes have recently emerged as a useful strategy for organic synthesis using visible light as a mild way to modulate chemical reactivity. Photoacids are bench stable weak acids in the absence of light irradiation and only upon irradiation become strongly acidic and thus catalytically active. This presentation will discuss the development of a photoacid catalyzed acetalization reaction using 6-bromo-2-naphthol. The rection scope, various light sources, and preliminary mechanistic studies will also be discussed.

Fr. Gerald Buonopane

8.

Evaluation of Carbonyl Compound Formation from Methyl Linoleate in the Presence of Prolines

Viral Shah, Amber Chaudhary, and Fr. Gerald Buonopane*

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In the methyl linoleate (ML) oxidation path, carbonyl compounds form as secondary oxidation products via the scission of alkoxyl radicals. The 2,4-dinitrophenyl hydrazine (DNPH) assay test method is used to determine carbonyl compounds and total carbonyl content that result from methyl linoleate secondary oxidation products. DNPH and carbonyl compounds react to produce hydrazone complexes under acidic conditions. Derivatives of carbonyl compounds are then separated, identified, and quantified via the use of liquid chromatography ultraviolet detector (LC-UV) analysis. Experimentally, equivalent moles of mixtures ML and proline, ML and N-t-butyl carbonyl Dproline, ML and proline methyl ester, ML and NZL-proline methyl ester, and ML and hydroxyproline were weighed in separate glass vials. The closed vials were stored in a preset oven at 37°C for four days (day 1 to day 4). Samples were analyzed daily. Samples were pulled from the oven and cooled to room temperature on each of the four days of analysis. An acidic solution of DNPH solution was prepared in N, N-dimethyl formamide. Acetonitrile solvent was added to samples for extraction purposes. Sample solutions were vortexed and then centrifuged. The supernatant solution was separated and acidified DNPH solution was added to the supernatant solution for derivatizing carbonyl compounds. Samples were then stored in the dark for 30 min at room temperature. Samples were analyzed by LC-UV using an Agilent 1100 the system, LC C18 Column 150 mm X4.6 mm, flow rate 1.5 ml/min with a gradient of water and acetonitrile mobile phases and hydrazones were detected at UV wavelength 365 nm. The presence and amount of carbonyl compounds as formed from methyl linoleate were determined using linear regression analysis with the standard nonanal. A lower amount of carbonyl compounds resulted in sample mixtures containing methyl linoleate and proline. Proline and derivatives were found to inhibit the ML oxidation path.

9.

Evaluation of conjugated Diene and Hydroperoxide Products Formation from Methyl Linoleate in Presence of Prolines

Amber Chaudhary, Viral Shaw, Simran Kaur, and Gerald Buonopane*

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Food storage is a major challenge for food chemists because of a number of potential degradation processes, including lipid peroxidation. This peroxidation process is an explosive reaction and very difficult to control. Lipid radicals react with an oxygen molecule to create a lipid peroxyl radical, this lipid peroxyl radical creates another lipid radical, and numerous degradation products result causing deleterious effects to the quality of the food. The reaction continues until an antioxidant ends the cycle.1 Intermediate compounds of the peroxidation reaction are very harmful, such as lipid hydroperoxides and conjugated dienes which are linked to many diseases.2The aim of this study is to use the amino acid proline to lower the concentration of lipid hydroperoxides and conjugated dienes produced. Proline, a non-essential amino acid, and a necessary part of collagen has been shown to have an antioxidant effect.3 In this experiment the ability of proline and some of its derivatives to decrease the concentration of lipid hydroperoxides and conjugated dienes will be determined. The prolines will be mixed with the lipid moiety methyl linoleate and kept in an oven at body temperature for a span of five days. To determine the effectiveness of the prolines at decreasing the concentration of the lipid hydroperoxides and conjugated dienes analysis via UV-Vis spectroscopy will be used. It is expected that the concentration of lipid hydroperoxides and conjugated dienes will decrease with the presence of the prolines. It is also expected that the different derivatives of proline will have varying effects on the concentration of the lipid hydroperoxides and conjugated dienes.

Dr. Jacob Goldsmith

10.

Where Art and Science Meet: First Experiments on Mocha Diffusion

Diana Malenkova and Jacob Goldsmith*

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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.

Dr. Sergiu Gorun

11.

Anchorable Fluorinated Phthalocyanines for Photodynamic Inactivation and Detection

Mary Chiọma Okorie, Ayuni Yussof‡, Tinchun Chu‡*, and Sergiu Gorun*

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

Phthalocyanines (Pcs) are a class of photosensitizers that can generate singlet oxygen ($^1O_2$), which decays to form reactive oxygen species (ROS), including hydroxyl (HO·) and superoxide radicals (O_2 ·) using visible light. These radicals target non-specific C-H bonds. Microorganisms thus cannot develop resistance to ROS attack. Organic photosensitizers self-destruction is a hurdle to practical applications such as catalysis and photodynamic therapy, but the hurdle can be resolved via Pc fluorination.1 A functionalized fluoro Pc, F48H7(COOH)PcZn was purified through column chromatography and its identity verified characterized by UVVis, HRMS and 19F NMR spectroscopy. Preliminary experiments reveal its antibacterial activity in DMF/ H2O solutions. Control experiments are currently underway to determine the stability and presence of the PC in a biological environment. The coupling of the Pc with branched poly-lysines was attempted but found to be not favorable thus far. The aim of this coupling, enhancement of the bioavailability of the photosensitizer via higher water solubility will be explored next by modifying the benzoic acid precursor starting material. An additional route was explored to see the conjugation of the photosensitizer with an amino-functionalized silica gel. In effort to anchor the Pc on solid supports for the purpose of detection of phenolic antibiotics in any media. Efforts are currently underway to develop and explore the conjugation of the Pc functionalized silica gel.

12.

Synthesis, Structures and C-H Oxygenation Reactivity of Perfluoroalkyl Iron Phthalocyanines

Mufeda Zhort and Sergiu Gorun*

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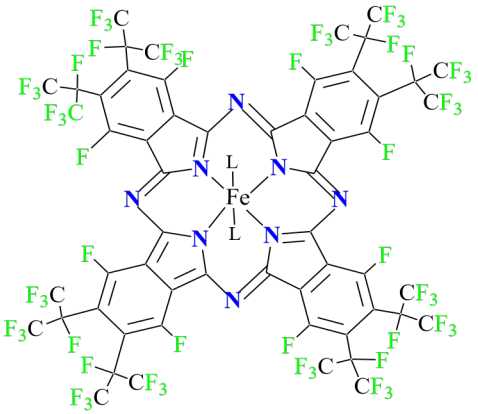
New perfluoroalkyl substituted perfluoro iron(II) phthalocyanines, $F_{64}PcFeL_2$, are electron deficient, low-spin, exhibit no Pc C-H bonds, are soluble in organic solvents, and, for L = H_2O, catalytically oxygenate cyclohexane with both t-butyl hydroperoxide and air without decomposing. The electron deficient [$F_{64}PcFe$] complexes exhibit stability, solubility and structural features desired for catalysis. A central hydrophilic region within a superhydrophobic cavity allows H_2O coordination and provides H-bonding pathways that contribute to the formation of parallel columnar stacks in the solid-state. The cobalt complex, [$F_{64}PcCo$], unlike its isostructural Zn analogue, and unlike the isoelectronic, but planar $F_{16}PcCo$, catalyzes the aerobic removal of H atoms from a -CH_3 group.

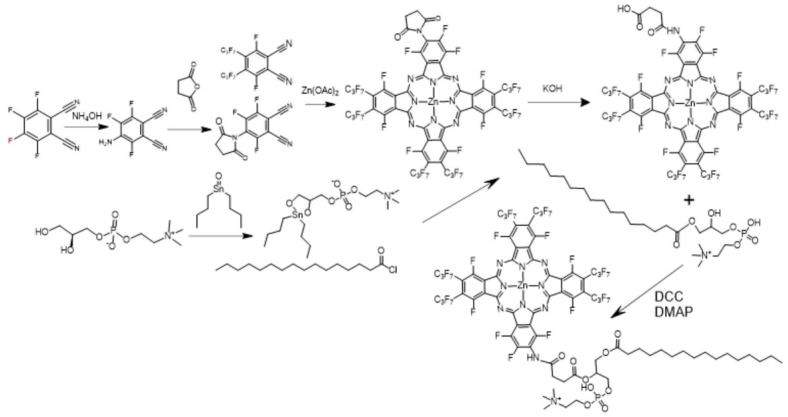


13.

Liposomes from Fluorinated Metal-Centered Phthalocyanine Phospholipid

Anthony Nesturi and Sergiu M Gorun*

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



A variety of metal-centered fluorinated phthalocyanins have been synthesized in our group1, but only a few attempts have been made to increase their bioavailability2. F64PcZn and Cu have very low water solubility, making them impractical for biological systems. Headway has been made in attaching F51PcZn to phospholipids, using a convergent synthesis method3. The amino precursors were obtained in 60-80% yiled by reacting tetrafluoro phthalonitrile with ammonium hydroxide, followed by the protection of the amine with phthalic or succinic anhydride. The protected precursors, obtained in 40-60% yields, form PcZn (30-40%) using microwave radiation. Coupling a phospholipid with F51PcZn will follow. These PcZn-lipids, which exhibit an encapsulated Pc, will be compatible with biological environments. The Pc, consistent with previous reports4, is expected to remain active. The covalent bond between the Pc and a phospholipid will facilitate the liposomal stability and formulation.

Dr. James Hanson

14.

Synthesis of Star Polymer Structures of Sulbactam Acid, a β-Lactamase Enzyme Inhibitor

Daniel Goldman and James Hanson*

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Antibiotic multi-drug resistance is a major challenge today in the medical management of infectious diseases. The need exist to moderate drug resistance of mutated bacteria as well as drug side effects. The goal of this synthetic project is to develop a small library of biodegradable star polymers conjugated to the β-Lactamase inhibitor, sulbactam acid. The core first chemistry will involve the esterification of sugar alcohols with glutaric anhydride via a ring opening reaction to form a multi homo-arm structure with terminal carboxylic acid groups. Sulbactam acid is then functionalized to an acyl chloride and then coupled to the terminal end of each homo-arm forming an anhydride linkage. The methodology produced finish products with various yields given temperature, solvent and reaction time conditions.The implications of star polymers are improved targeted drug delivery that will result in pharmacological efficacy, absorption, distribution, metabolism, excretion and diminish the effects of drug resistance in the treatment of infectious diseases.

15.

Cationic Porphyrins via Click Chemistry

Usha Kalra and James E. Hanson*

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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 excesses of alkylating agents. We have explored the use of "click chemistry" as an alternative method for the preparation of tetracationic porphyrins.

16.

Formulation and Evaluation of Antibiotic Microspheres against Gramnegative *Escherichia coli* and Gram-positive *Staphylococcus aureus*

Miguel Medico, Ayuni Yussof ‡, Tin-Chun Chu‡*, Dr. James E. Hanson*

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

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, antiiflammatory, 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.

17.

Evaluation of Self-Cleaning Surfaces

Edrice Sediq, Brandon Pineda, Abdul Azeez, and James E. Hanson*

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Self-cleaning surfaces were prepared from a siloxane-epoxide coating material which incorporated the volatile solid ammonium bicarbonate to generate surface roughness and increase hydrophobicity and a perfluorinated phthalocyanine on a titanium dioxide support to provide catalytic photo-oxidation. Self-cleaning characteristics were evaluated using the dyes methyl orange and crystal violet as test compounds. Catalytic photo-oxidation through irradiation of the films stained with the dye solutions was analyzed through UV-VIS spectroscopy. It was observed that with ~240,000 lux of light intensity and irradiation times of 0 min, 20 min, 40 min, and 60 min there was degradation experienced on the surface. The greater time spent under the light source the more degradation was experienced as expressed by visible color aging of the films and UV-VIS decreases in absorbance. The increase in hydrophobicity contributed by the ammonium bicarbonate surface roughness was observed during visible "roll-off" of the prepared dye solutions of crystal violet and methyl orange. To observe the "roll-off" effect the films were positioned at 0^o, 30^o, 60^o, and 90^o and sprayed with the prepared stains using a 250 µl blunt-tip syringe. UV-VIS analysis was performed on the films to confirm the "roll-off" phenomena observed. It was determined that slides treated with ammonium bicarbonate experience "roll-off" beyond 0^o. Future directions include experimenting with different angles to see if the hydrophobicity of the ammonium bicarbonate treated films can hold up with angles closer to 0^p and further irradiation testing to see the extent of dye degradation on the films.

Dr. Yuri Kazakevich

18.

The Influence of Pressure and Shear Heating Influencing Retention in Reversed-phase Chromatography

Timothy Nowak, Alexey Makarov, and Yuri Kazakevich*

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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 (3μm, 5μm) 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 shear 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.

Dr. Stephen Kelty

19.

Structural Composition of Stacked Alternating Y_2O_3/ZrO_2 Multilayers Using Classical Atomistic Modeling

Logan Ockershausen and Dr. Stephen Kelty*

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Yttria Stabilized Zirconia (YSZ) has been of great technological interest due to its ability to act as a solid electrolyte for use in advanced battery technologies, Solid Oxide Fuel Cells, and many other uses. A key aspect of using YSZ is to stabilize the cubic form of zirconia. Many preparative methods have been used to introduce yttrium atoms into the zirconia lattice. Recent efforts to do this involve preparing very thin alternating atomic layered deposited (ALD) layers of zirconia (~1.0 nm) and yttria (~0.1 nm) followed by annealing. In this project, computational methods are used to model the dynamical processes of such a preparative method. We seek to help determine the propensity of the Y atoms to uniformly distribute into the zirconia layers and formulate stabilized YSZ in models based on the ALD method versus the sputtering method which generates one thick layer of YSZ. The MD simulations will be carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software package available from Sandia Laboratories on 8- and 32-core parallel processor servers. Classical potentials using the Buckingham potential will be used for the project which have been developed in the Kelty Research Group. The investigations will focus on several structural details of ALD and/or sputter prepared films, including phase segregation, crystallinity, and diffusion rates of Y into the zirconia layers.

Dr. David Laviska

20.

Progress in the Development of a New Thematic Sequence of Laboratory Experiments for an Organic Chemistry Course based on the Tenets of Green Chemistry, Stewardship, and Sustainability

Kyle G. Otto and David A. Laviska*

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As previously reported, several undergraduate members of our research group have piloted and/or modified green(er) experimental protocols taken from the literature for implementation in organic chemistry teaching laboratories. Under the auspices of the new Green Chemistry, Stewardship, and Sustainability Program (GCSSP) at Seton Hall University, we are now in the process of developing curricular materials that address one or more of the title concepts. In thinking about helping students make connections between different classes of reactions in organic synthesis, we propose that a common starting material (or derivative) can serve to underline the relationships between broad reaction classes (oxidation/reduction, acid/base catalysis, etc.), and to this end, a thematic sequence of laboratory experiments based on the renewable molecule furfural is currently being developed. Beyond the details of the laboratory protocols themselves (tenets of green chemistry, etc.), we want students to think broadly about concepts like stewardship of the environment and sustainability, so questions and discussion points relating to the 17 United Nations Sustainable Development Goals are being incorporated into pre-lab and post-lab exercises. This talk will focus on connections between course concepts, experimental details, and global concerns addressed by many of the U.N. SDGs.

21.

Progress on the Development of Greener Protocols for Synthesizing Substituted Quinoxalines for use as Cyclometallating Ligands in Late Transition Metal Complexes

Anthony Rodriguez and David A. Laviska*

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Quinoxalines, or benzopyrazines, are a class of heterocyclic aromatic compounds that are currently employed in industry as dyes and building blocks for many pharmaceutical drugs. Our group is interested in the synthesis of these compounds for possible use as mono-, di-, and tridentate ligands in late transition metal complexes. In order to explore the physical and chemical properties of 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 eight ligands in good-to-excellent yield and high purity using these protocols. These ligands fall into either the 2,3-diphenyl, 2,3-difuranyl-, or 2,3-dipyridylquinoxaline categories, and after making the unsubstituted versions of these molecules, we broadened the scope to include substituents like fluorine and trifluoromethyl groups. Herein, I will discuss the following: details of our synthetic methodology which highlights the use of microwave heating that drastically reduces the reaction time, the specific quinoxaline analogues we have synthesized, and the transition metal complexes made thus far with our ligand library.

22.

A Greener Approach to the Synthesis of a Family of Benzoquinoxalines for use as Ligands in Transition Metal Complexes

Andi-Kaye M. Walters and David A. Laviska*

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New materials for use in state-of-the-art organic light emitting devices (OLEDs) are being vigorously researched, and organometallic complexes of iridium and other late transition metals hold great potential due to their highly desirable photophysical properties. While the choice of transition metal is a critical determinant of emissive properties, it is the surrounding ligand system that affords the ability to fine tune to desired wavelengths, and therefore colors, of light production. Polyaromatic heterocycles such as quinoxalines have been extensively studied when used as bidentate ligands in tris-ligated (homo- or heteroleptic), octahedral metal complexes. Our group has developed an improved, greener synthesis of these molecules and other related systems such as benzoquinoxalines – a slightly larger molecule with five aromatic moieties. As a family of ligands, the benzoquinoxalines have been significantly less studied, but represent an extension of conjugation that may lead to interesting emissive properties. To date, we have successfully synthesized a family of four benzoquinoxalines and started utilizing them as ligands in complexes of iridium. Details of the synthesis and characterization of the ligands, an evaluation of the alignment of the syntheses with the tenets of green chemistry, and a system-oriented concept map extension (SOCME) describing the broader context for this research project will be presented.

23.

Greener Synthesis of Polyaromatic Ligands based on a 1,2-Diimine Framework

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The development of new materials for use in fluorescent and phosphorescent organic light emitting devices (OLEDs and PHOLEDs) continues to inspire interest in novel organometallic complexes that might have potentially unique photophysical properties. Our group has been working on applying the tenets of Green Chemistry to existing literature protocols for various coupling reactions in order to reduce additives and by-products while yielding bi- and polyaromatic molecules for use as ligands in transition metal complexes. Utilizing a high-yielding variation of a Schiff base condensation reaction, we are attempting to synthesize a family of ligands based on a 1,2-diimine motif. Starting with benzil (a 1,2diketone) and two equivalents of aniline, we have synthesized 1,2-tetraphenylethane-1,2diimine, though yields have not been reproducible and we are still in the process of optimizing the synthetic scheme, including microwave heating parameters. It appears that both electronic and steric variables are important in determining yields of products and may limit the types of reactants that can be successfully used. Therefore, a spectrum of reactants have been chosen that will yield a family of ligands based on the 1,2-diimine motif, as well as inform our understanding of the potential limitations of these reactions.

Dr. Wyatt Murphy

24.

Synthesis and Characterization of Biodiesel using Microalgae as Sustainable Triglycerides Source

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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. The project shows the feasibility of the biodiesel production process by investigating its optimization and proving that microalgae are a useful source of oil for the synthesis of biofuel. Chlorella sp. algae are used in the first stage of the research project and were cultivated in Carolina Alga-Gro Freshwater Medium and in BG-11 Medium in the McNulty greenhouse. MiracleGrow fertilizer containing Nitrogen and Phosphate was added to boost algae growth. Moreover, DI-water was found to be unable to sustain algae. Algae growth was monitored by taking the absorbance at 600 nm using UV-Vis spectroscopy and already showed promising results early on in the first stage of this young project. This data also serves as reference for future steps where parameters affecting algae growth and triglyceride quantity will be further investigated. The oil extraction method and transesterification reaction will be based on selected research experiments from literary sources, allowing the synthesis of biodiesel to be intensively studied with the goal of optimizing this process. Furthermore, the project aims to outline a three-year research proposal for biodiesel research at SHU, as part of the Green Chemistry Initiative and the much-needed scientific research in this area. Further studies on biodiesel production and alternative fuel sources will encourage the largescale production of biofuels and will aid in the global transition to more sustainable and environment-friendly energy sources.

25.

Microwave Assisted Synthesis and Photophysical Analysis of ROS Generating Iridium(III) Complexes

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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 $[Ir(ppy)_2(4,4'\text{-dicarboxy-}2,2'\text{-bipyridine-}]Cl$ and $[Ir(2phenylquinoline)_2(bathocuproine)]Cl$. 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 COrrelated 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.

26.

Optimization of Microwave Synthetic Conditions for [Ir(ppy)2(2,2'-bipyimidine)](PF$_6$) and [Ir(ppy)2(2,2'-bipyridine)](PF$_6$)

Nataly Areosa Suarez, Florian Balan, Allyson Dixon, and Wyatt R. Murphy*

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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 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. We have spent the past two years optimizing efficient, high yield syntheses of [Ir(ppy)2(2,2'-bipyimidine)](PF6) and [Ir(ppy)2(2,2'-bipyridine)](PF6) (ppy = 2-phenylpyridine) as test examples. After, establishing a concrete procedure using the microwave, and producing a sufficient amount of these products, further examination were conducted including determination of the radiative quantum yields via relative methods and radiative lifetime via single photon counting.

27.

Microwave Synthesis and Photophysical Characterization of Novel Heteroleptic Iridium Complexes Containing Polyaromatic C^N and N^N ligands

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A novel series of heteroleptic, cationic iridium complexes, with purpose to serve as potential components of OLED and LEC devices, were synthesized through a green, combinatorial based approach. We have utilized a microwave reactor in order 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 iridium (III) complexes using microwave heating, resulting in drastically reduced preparation times compared with conventional heating as reported in the literature the C^N-cyclometalating ligands, quinolone based, and the N^N dative ligands, cuproines and phenanthroline derivatives, were varied with the purpose to assess the effect of structural differences, specifically steric crowding, on functionality of the complex. The general formula being $[Ir(pq)_2(N,N)]^+$ (ppy = 2-phenylquinoline; N,N = cuproines).The importance of functionalization of ligands can be explained by the nature in which overall electronic properties are manipulated; the stabilization of the HOMO through the addition of electron withdrawing groups and the destabilization of the LUMO with the addition of electron donating groups. Differences in photophysical and electrochemical properties of the complexes were assessed through UV-VIS, fluorescence, and cyclic voltammetry. High radiative quantum yields and long lifetimes indicated efficient phosphorescence. Structural analysis and extent of steric crowding of various ligands was conducted with the use of standard H NMR as well as 2-D NMR.

28.

Green Chemistry, Stewardship, and Sustainability Program at Seton Hall University

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The Green Chemistry, Stewardship, and Sustainability Program (GCSSP) was recently approved by Dean Peter Shoemaker to promote and educate students about the title concepts. This program grew out of the Green Chemistry Initiative (GCI) - initially established in 2018 with unanimous departmental approval - to confront potential overcrowding of organic chemistry laboratories due to increasing student enrollment. The first major goal was to convert the CHEM 2315-16 lab sequence to safer, greener protocols; this successful effort resulted in significantly lower operating costs per student due to fewer/cheaper reagents and generation of less waste. Further, the students are now systematically introduced to the principles of green chemistry, a major initiative for the American Chemical Society. Ultimately, the GCI informed the decision to include microwave reactors in the newly constructed lab SC-116, initiated new research efforts in green chemistry, and took over management of SC-306, formerly the Center for Applied Catalysis. GCSSP members have developed strong connections within the chemical community, including Beyond Benign and the American Chemical Society, and are serving as program chairs for meetings, leading educational efforts, and presenting talks based on green chemistry and systems thinking. Two courses are currently in development for Spring 2022 – a CORE III course on Stewardship and Sustainability and a course in Green Chemistry for chemistry majors and minors. The GCSSP will present a Great Minds Symposium in August, and CHEM 1001 (Chemistry and the World Around Us) now has a significant green chemistry focus. These initiatives and future plans will be presented.

29.

Novel Heteroleptic Iridium Complex for PDT

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Photodynamic therapy is a non-invasive, pharmaceutical method utilizing lightactivated reactions between a complex called a photosensitizer and molecular oxygen (^{3}O2). Its medicinal use is based on the generation of cytotoxic singlet oxygen (ROS) and its ability to manage drug activity at a targeted area. A novel library of heteroleptic iridium (III) complexes with important photophysical properties were synthesized to act as photosensitizers. Cationic heteroleptic iridium complexes are very photostable and manifest large radiative quantum yields and long excited state lifetimes making them useful as photosensitizers. These qualities can be further enhanced by selection of cyclometallating and dative ligands. Microwave-assisted techniques address several issues of chemical sustainability present in more traditional methods and promote the twelve principles of green chemistry. In using one-pot microwave synthesis, the process eliminates intermediate steps and promotes lower energy input, the minimization of waste, the maximization of atom economy, and the elimination of the use of hazardous synthesis techniques. Dr. Murphy's previous research[4] regarding organic molecules forming complexes with ruthenium and rhenium is basis of the design of the novel library of iridium complexes. The general form of said complex includes a dative ligand (N^N) and a cyclometallated group (C^N). Ideally for photodynamic therapy, a red-shifted, and thus more easily penetrating complex with long excited state lifetimes and large quantum yields is desired. Antimicrobial photodynamic therapy has been found to be a promising method of treating several pathogenic fungi[6]. With the attachment to a mitochondrial targeting peptide, an iridium complex has the potential to generate cytotoxic singlet oxygen, thus killing the fungus. A water-soluble iridium complex has been synthesized, via the selection of (2-phenylpyridine) and dicarboxybipyridine ligands with the use of a chloride counter anion, which will be conductive to the environment of a living organism.

Dr. David Sabatino

30.

Synthesis, Characterization, and Biological Evaluation of Polyarginine Derived Bone-Targeting Peptides

Gina L. Antuono,[1] Jenny Zilberberg[3], Jessica Cottrell[2], and David Sabatino[1]

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Many cancers are susceptible to metastasis within the bone extracellular matrix largely due to the interactions of adhesion proteins found on the surface of bone cells, such as osteoblasts and osteoclasts. By targeting these cell surface adhesion proteins (N-cadherin, E-cadherin, b-catenin, periostin and fibronectin) with short-interfering RNA (siRNA), the adhesive interactions of malignant cells, such as tumors, are diminished, rendering them susceptible towards treatment. In this presentation, a selected osteoblast-targeting peptide (Ser-Asp-Ser-Ser-Asp, SDSSD) which selectively binds to periostin on the cell surface of osteoblasts, is functionalized with polyarginine sequences of varying lengths (6-12 Arg), for facilitating selective osteoblast cell uptake of siRNAs that can silence cell adhesion proteins (e.g. N/E-cadherin, periostin, fibronectin) involved in tumor metastasis that can originate or migrate to the bone (e.g. prostate, breast, and multiple myeloma). This work will highlight peptide and siRNA solid phase synthesis methods, LC/MS characterization and conditions for formulating peptide-siRNA complexes for molecular cell biology applications in osteoblast cells and in co-culture with tumors. In this manner, our gene therapy approach aims to target bone tumors that may be difficult to treat due to their protective adhesive interactions with bone.

31.

Rational Design, Synthesis, Characterization and Biological Evaluation of Cancer-Targeting Immunostimulatory Peptide

[1]Nelson Casanova, [2]Rachel Montel, [2]Keith Smith, [1]Zena Karem, [2]Constantine Bitsaktsis, [3]Dante Descalzi, [3]Robert Korngold, and [1]David Sabatino

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With the advent of cancer immunotherapy and synthetic biologics, there has been a steady decline in the incidence of cancer. Despite this trend, there is still an anticipated 1,898,160 new cancer cases and 608,570 cancer deaths projected to occur in the United States in 2021 according to the American Cancer Society. Therefore, the need for creating more effective treatment options are still in high demand. In this presentation, several cancer-targeting immunostimulatory peptides are presented as activating epitopes of the Natural Killer (NK) and Cytotoxic T cell Lymphocytes (CTLs). These synthetic biologics have independent immunostimulatory activities towards their target NK and CTL activating receptors; however, with restricted duration of action and limited immunotoxicity towards tumors. Therefore, we hypothesized that a combination of these peptides in a single molecular motif may induce enhanced activation of NK and T cells' effector functions enabling tumor cytolysis compared to individual peptide or cell line treatment. The peptide motifs range from linear, dimer and trimer peptides incorporating multiple epitopes for synergistic NK and CTL activation for tumor immunocytolysis. The multiepitope immunological inducers have the ability to provoke multipeptide-specific cytotoxic responses in solid and hematological tumors thereby raising their clinical potential. Using Fmoc-Solid Phase Peptide Synthesis, we have generated a library of multiepitope peptides most of which were purified and characterized by RP-LC/MS and UV/Vis spectroscopy. Using flow cytometry, the preliminary data confirmed that the linear peptides bind and activate, NK92-MI cells which translated into cancer immunotherapy effects *in vitro* and *in vivo*. We anticipate the specific binding of the peptide motifs to multiple activating receptor targets will provide the best candidates for optimizing our cancer immunotherapy approach.

Dr. Nicholas Snow

32.

Analysis of Sweet Basil and Its Essential Oils by Gas Chromatography

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Basil, also known as *ocimum baslicum*, is a culinary herb that has been known to have many health benefits, such as the reduction of oxidative stress, blood sugar regulation, heart disease prevention, and many more. This is due to its many antioxidants, like eugenol, estragole, and others that are present in its essential oils. Gas chromatography (GC), gas chromatography-mass spectrometry (GC-MS) and comprehensive twodimensional gas chromatography-time of flight mass spectrometry (GCxGC-ToFMS) were used to separate the various components of sweet basil oil. Commercially available basil and basil oil samples were examined along with samples extracted from plasma treated and non-plasma treated basil plants. Basil plants were extracted using simple solvent extractions and steam distillation to provide the oil components. The effects of different instrumental techniques, extraction techniques and pre-treatment of the plants on the observed chemical profiles of the essential oils will be discussed.

33.

Development of Various Gas Chromatography Methods to Detect Analogs of Fentanyl

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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.

34.

Qualitative Analysis of Clove Oil Using Gas Chromatography and Mass Spectrometry

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Gas chromatography is a method of separation in which substances are passed through a stationary and mobile phase to distinguish the components. When used in conjunction with mass spectrometry, these components become easily identifiable. In this research, gas chromatography was 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 three methods of gas chromatography – Gas Chromatography, Gas Chromatography-Mass Spectrometry, and Gas Chromatography x Gas Chromatography-Mass Spectrometry – separation of the components of clove oil was performed. This qualitative data was then used to compare the three methods of chromatography in their ability to separate and distinguish compounds from clove oil. The chemical makeup of clove oil, viewed through the lens of each of these three instruments, will be discussed in this presentation.

35.

Polyol-induced Extraction of Glucocorticoids from Water and Determination using UHPLC-MS/MS

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Polyol-induced Extraction was used for the extraction and analysis of glucocorticoids.
Polyol-induced extraction is an extraction technique developed and patented by Sowa, Murphy, and Deshpande at Seton Hall University, as a technique for extracting water from mixtures with polar organic liquids or the reverse. 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 was used as a mass separating agent in the extraction of glucocorticoids from water into polar organic solvents. Glucocorticoids were extracted by polyol-induced extraction and will be analyzed by UHPLC-MS/MS. MRM transitions were evaluated for each compound for the detection and quantification. Percent recovery and partition coefficients, accuracy, precision, limit of detection and limit of quantification were determined for each glucocorticoid. The glucocorticoids under this study include beclomethasone, cortisone acetate, prednisone, hydrocortisone, prednisolone, dexamethasone, fludrocortisone acetate and methyl prednisolone. Extraction optimization was performed to determine optimum extraction condition by studying three different temperature condition, extraction time and amount of polyol, leading to the extraction being performed with 1:1 ACN/Water mixture using Glycerol as a phase separating agent.

36.

Qualitative Analysis of Spearmint Essential Oil Using Gas Chromatography and Mass Spectrometry

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Gas Chromatography is used as a separation technique in which substances partition between the stationary phase in the column and the mobile phase. The Gas Chromatography-Mass Spectrometry apparatus serves as a segregation method to separate components of a mixture, and then can investigate those components at the molecular level. In this research, we will be working with samples of spearmint oil. Spearmint oil is used in essential oil diffusers, cooking, and skincare, and has many health and antioxidant benefits. Using gas chromatography (GC), gaschromatography-mass spectrometry (GC-MS), and comprehensive two-dimensional gas chromatography (GCxGC-MS) qualitative data on the separation and components of of spearmint oil determined on each of these instruments will be discussed. This data will be used to compare and contrast the instruments and to provide insight into the major and trace components of commercial spearmint oil, and to discuss the distinctions between the three instruments, as seen from the data.

37.

QuEChERS Extraction of Glucocorticoids from Water and Determination using UHPLCMS/MS

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QuEChERS is an extraction method which involves two main steps: a liquid-liquid extraction and a dispersive solid phase extraction (d-SPE) which is a cleanup step. This two-step process begins with the analytes of interest being extracted first, followed by the d-SPE cleanup step where potential interferences are removed. The original methodology of QuEChERS involved analyzing veterinary drugs in animal tissue, but in this work it was utilized to identify glucocorticoids in water following the procedure developed by Schmidt at Seton Hall University. In QuEChERS extraction, acetonitrile is added as an extraction solvent to the homogenized sample and then centrifuged with the addition of buffering salts to extract the analytes of interest. Glucocorticoid extraction was performed in 1:1 $MgSO_4$/NaCl mixture using aqueous sample (mixture of all eight steroids) and ACN. The focus of this work was to utilize QuEChERS extraction as an effective technique in determination of glucocorticoids. Glucocorticoids were extracted by a previously optimized QuEChERS extraction method and were analyzed by UHPLC-MS/MS using multiple reaction monitoring for quantitation. The data will be evaluated by comparing it with previous research done using GC-MS/MS for detection.

Dr. Gregory Wiedman

38.

Formulation of Antifungal Peptide Against Cryptococcus Neoformans

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Cryptococcus neoformans is an antibiotic resistant pathogenic fungus which can present in its most severe form as meningitis. This fungus is most concerning for immunocompromised patients. The P4-ATP-flippase membrane protein of Cryptococcus is responsible for translocating phosphotidylserine (POPS) across the membrane from the extracellular side to the intracellular side. Lipidated peptides based on the CDC50 loop region of the flippase were developed which target the flippase protein. MIC values of generation two peptides were half the concentration of the MIC value of generation one peptide against the ΔCDC50 mutant.

39.

Photomelittin: A Photoisomerizable Membrane Active Peptide

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Melittin, the key component of honey-bee venom, is an α-helical lytic peptide toxin that permeabilizes the cell membrane by forming membrane spanning pores. The central proline residue (P14), which is critical for melittin's activity, induces a bend in its helix. Proline can readily form the *cis*-Xaa-Pro bond. This enables proline to facilitate structural changes within a larger peptide structure. In this work we propose that P14 can be studied by utilizing a molecular photoswitch as a proline proxy. Azobenzene is a photoisomerizable molecule that has recently been incorporated in a variety of biological applications including as a β-turn mimic. We hypothesize that the P14 residue of melittin can be substituted for an azobenzene amino acid (Z14) to create a similar helix-hinge-helix effect that has the potential to allow the activity of melittin to be controlled with light. A melittin analog, photomelittin, has been synthesized by solid phase peptide synthesis. Upon excitation with UV light photomelittin isomerizes from the *trans* to the *cis* isomer and can be converted back to the *trans* isomer by irradiating with blue light. The P→Z substitution was found not to alter the secondary structure and only slightly reduces the membrane binding affinity. Photomelittin is less membrane active than melittin at lower concentrations but is also less hemolytic. Moreover, *trans* and *cis* photomelittin have been found to display concentration dependent differences in activity.

40.

Investigating the Antifungal Susceptibility of *Candida auris*

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Candida auris is a recently emerged fungi that is responsible for causing candidemia, also known as a bloodstream infection (BSI). First discovered in 2009, numerous cases have been reported in five different continents[1]. Besides its persistent virulence on nosocomial surfaces, rapid multi-drug resistance (MDR) has been observed in *C. auris*. This presents a particular concern to immunocompromised individuals, such as those undergoing chemotherapy and organ transplant surgery. There are currently four classes of antifungals available for clinical use: azoles, polyenes, echinocandins, and flucytosine. Despite its phylogenetic divergence from other infectious *Candida* species[2], *C. auris* has displayed similar levels of reduced susceptibility to each of these classes. Considering the alarming rise in MDR among fungal pathogens, understanding the mechanisms of resistance is of paramount importance in the development of effective antifungal treatments. We present the synthesis of a light-activated metal-peptide conjugate as a fungal growth inhibitor. Conventional solid phase peptide synthesis (SPPS) was used to synthesize a membranetargeting peptide, MIASHLLAYFFTELNGKPILFF-NH_2, which was subsequently labelled with an iridium complex, [Ir(2-phenylpyridine)$_2$(4,4'-dicarboxy-2,2'-bipyridine)]Cl. The peptide, designed on the primary structure of hexokinase II (HKII)[3], serves to target mitochondria, while the Ir portion of the complex generates singlet oxygen ($^1O_2$) upon exposure to visible light. Minimum inhibitory concentration (MIC) assays were conducted against multiple strains of *C. auris* with amphotericin B, caspofungin, and itraconazole. The experimental breakpoint values were significantly higher than the reported breakpoint values from the Center for Disease Control (CDC), demonstrating increased tolerance to these antifungals. Further MIC assays will be conducted to examine the efficacy of the Ir-peptide hybrid.

41.

Iridium Mitochondrial Targeting Peptide to Treat Drug-Resistant Fungal Infections

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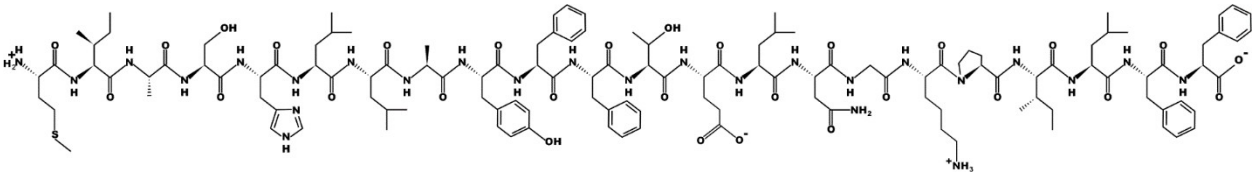

Mitochondria are essential organelles that directs a cell's energy production, signal transduction, and metabolic regulation. The mitochondria hold a crucial role in physiological and pathological processes, qualifying them for studies as a potential therapeutic target for the treatment of various diseases and infections. Mitochondrial penetrating peptides (MPPs) identify as cationic and lipophilic, facilitating permeation of the hydrophobic mitochondrial membrane. Peptide-based mitochondrial agents are considered biocompatibility and have straightforward synthesis, that would facilitate modification with therapeutic cargos. A mitochondrion targeting sequence with cell penetrating peptide, MIASHLLAYFFTELNGKPILFF (Figure 1), attached to phosphorescent Ir(III) complex is hypothesized, by Dr. Wyatt Murphy and Dr. Gregory Wiedman, to eradicate infectious cells utilizing photodynamic therapies (PDT). The iridium peptide hybrid (IPH) posed complications when attaching the iridium complex to the MPP, including crossing of functional groups, low solubility, and steric hinderance due to cationic charges. Iridium complexes have an important photophysical property and by attaching them to a mitochondrial targeting peptide sequence it could potentially eliminate fungi species such as *Candida glabrata*. This fungal species possesses innate and acquired resistance against antifungal drugs, due to its ability to modify ergosterol biosynthesis, mitochondrial function, and antifungal efflux. *C. glabrata* is a source of morbidity, triggers chronic pain or discomfort limiting nutrition intake within the immunocompromised and elderly patients. The IPH was synthesized on a CEM Discover microwave peptide synthesizer under the conditions as described by the manufacturers. Synthesis required the use of a solid support, resin beads with a reactive amide group, which the peptide covalently attached to throughout the entire process. For the analytical components such as HPLC and mass spectroscopy tests, the data is currently pending and will be completed soon. HPLC testing will include a gradient of 0.1% concentration of formic acid dissolved in H_2O and acetonitrile. In the future, minimal inhibitory concentration (MIC) and hemolysis assays will be utilized to determine the effectiveness and toxicity of the overall compound against *C. glabrata*. Positive and negative controls will regulate the results generated by the IPH and its effect on *C. glabrata.* In conclusion, the IPH has potential to eradicate infectious fungal cells and in prospective to do the same with other types of bacteria and fungi.

42.

Development of Rifampicin-Binding and Rifabutin-Binding Aptamers for a Quick and Easy Therapeutic Drug Monitoring Method Toward Tuberculosis

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Rifampicin and Rifabutin are antibiotics used to treat several types of bacterial infections, including tuberculosis (TB). Rifampicin or Rifabutin are known to produce hepatic, renal, hematological disorders, and convulsions by inhibiting DNA-dependent RNA polymerase activity and forming a stable complex with the enzyme. To detect the amount of the antibiotics in a patient, analytical methods using High Performance Liquid Chromatography tests are available. However, the tests are expensive and inaccessible to third-world countries, where TB are prevalent. Additionally, the need for Therapeutic Drug Monitoring is crucial for understanding drugs that are effective, yet toxic, for fighting antimicrobial resistance, and for dosage adjustment as a result of drug-drug or food-drug interactions. The low technology assays, such as thin layer agar tests have high turnaround time. Using the Systematic Evolution of Ligands by Exponential enrichment (SELEX) process, we develop aptamers from nonspecific 40-mer Deoxyribonucleic Acid (DNA) library to interact with its target, Rifampicin or Rifabutin, which provide a simple method of detection. Once these selective aptamers are obtained and throughout the process, various scientific assays, such as Polymerase Chain Reaction (PCR), gel electrophoresis, Graphene Oxide, Fluorescence assays using Plate reader, and Circular Dichroism (CD) spectroscopy were performed to evaluate aptamer-Rifampicin or aptamer-Rifabutin binding. Discovering molecules that bind with Rifampicin-labeled beads more than unlabeled beads will provide insights on the selectivity and specificity of the aptamers. Further modification and optimization will lead to a molecule that can be used for therapeutic drug monitoring with this devastating disease.

43.

Cryptococcus Neoformans and Plasma

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Cryptococcus neoformans (C. neoformans) are in a special category of fungi due to their radiotrophic qualities. Radiotrophic organisms tend to proliferate and grow better when exposed to radioactive conditions, and in the case of C. neoformans, gamma radiation. Since C. neoformans grow well in radioactive conditions, the question for this experiment was, how well would it grow when exposed to plasma? We attempted to study the effects of a 5.00 L helium fed plasma on *C. neoformans* to possibly derive factors that makes it thrive in radioactive conditions. Particularly, to shed more light on the role of melanin in the radiotrophic capabilities of C. neoformans. After culturing and plating melanized C. neoformans and non-melanized *C. neoformans,* both were treated with a 5.00 L helium fed plasma. The group counted the individual colonies of each plate to determine which type of culture, melanized, or non-melanized *C.neoforman* proliferated most under our designed conditions. The results showed that the non-melanized *C.neoforman* grew better than the melanized *C.neoforman* when treated with plasma and under our set conditions.

44.

Re-examination of Hold-up Time in Gas Chromatography

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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 (η), 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 put under a microscope 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.

45.

Finite Difference Studies of Peak Shapes, Numerical Extrapolations and Simulation Models of HPLC and GC Peaks in Chromatography: A Comparative Study

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Most phenomena in chromatography can be modeled with aims to improve performance or trends. Various modeling schemes with different degrees of complexity have been proposed to study chromatographic processes and to improve separation techniques. With increasing degree of complexity in the modeling of chromatographic processes, accuracy and computational time become important. For example, in gas chromatography (GC), it is possible to predict accurately the retention time under temperature programmed conditions, if the chromatographic retention behavior of a compound is known under isothermal conditions at different temperatures. Furthermore, simulation models present various capabilities, such as modeling the effects of pressure programming, column dimensional changes, serially coupled columns, and peak broadening. The aim of this study is to demonstrate how a novel VBA simulation in-house software compares with other HPLC and GC simulations programs such as EZGC, DryLab and other programs currently available online. In this work, chromatography data will be acquired for several compounds under the right conditions. We also intend to compare the separation performance and optimization in all simulation cases in order to better understand why a given operational mode perform better or worse than other readily available chromatography software. Results will be then compared with outputs from the readily available Restek EZGC simulation software as well as others, in order to better understand elution models and to predict chromatographic retention times. Obtained relationships are particularly useful, since predicted retention times can lead to rapid method development in chromatography by simplifying the selection of chromatographic parameters.