22nd Annual
March 2, 2024

Raymond N. Castle
Student Research Conference

UNIVERSITY of SOUTH FLORIDA
Department of CHEMISTRY

castleconf.org

In 2024, generative AI and large language models have become indispensable tools across science, scholarly writing, and everyday life. In scientific research, these technologies power breakthroughs in drug discovery, protein folding, and materials science by accelerating data analysis and hypothesis generation. In scholarly writing, they aid researchers in drafting papers, summarizing literature, and facilitating cross-disciplinary collaboration. Everyday life sees their pervasive influence through virtual assistants, language translation apps, and personalized recommendation systems, enhancing communication, accessibility, and user experiences. As of 2024, the seamless integration of generative AI and large language models continues to redefine how we explore the frontiers of knowledge, communicate ideas, and navigate the digital landscape. (written by Chat-GPT 3.5 given the prompt: write a short paragraph about the use of generative AI and large language models in science, scholarly writing, and everyday life as of 2024)

To generate the cover art Chat-GPT 3.5 was asked for a prompt: "Give me a prompt for DALL-E 3.0 that will make an image of a realistic bull doing chemistry experiments in a lab. Gold and green should be the main colors, the image should be elegant and professional but also very cool and artsy." This prompt yielded the following input for DALL-E that was used to generate the cover art: "A realistic bull, immersed in a chemistry experiment within a sophisticated laboratory setting. The ambiance is dominated by shades of luxurious gold and vibrant green, evoking elegance and professionalism. However, the scene is also imbued with a cool and artsy vibe, featuring avant-garde elements and artistic flourishes that elevate the image to a visually captivating level."

Cover Art: DALL·E 3

Cover Design: Guy W. Dayhoff II

22nd Raymond N. Castle Student Research Conference

Saturday, March 2nd, 2024

Department of Chemistry, University of South Florida

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Table of Contents

Agenda

Breakfast and Registration 09:00am - 09:30am
(CHE Breezeway and 1st Floor)

Oral Session A 09:30am - 10:50am
(CHE 303)

Oral Session B 09:50am - 10:50am
(CHE 217)

Oral Session C 09:50pm - 10:50pm
(CHE 302)

Poster Session/Competition 11:00am - 12:15pm
(CHE 101, CHE 102, & CHE 103)

Lunch 11:45am - 12:45pm
(CHE 217, CHE 302, & CHE 303)

Oral Session D 01:00pm - 02:50pm
(CHE 100)

Oral Session E 01:00pm - 02:50pm
(CHE 111)

Castle Introduction 03:00pm - 03:10pm
(CHE 100, Edward Turos, Ph.D)

Plenary Presentation 03:15pm - 04:00pm
(CHE 100, Sherri A McFarland, Ph.D)

Award Ceremony 04:00pm - 04:15pm
(CHE 100)

Chemistry Bowl 04:30pm - 05:30pm
(CHE 100 - Pizza & Games Hosted by Chemistry Society at USF)

Remembering Raymond N. Castle

Raymond N. Castle was born on June 24, 1916 in Boise, Idaho where he attended Boise High School and Boise Junior College. A 1938 graduate in Pharmacy from the University of Idaho, Southern Branch in Pocatello, he completed the M.A. degree in Chemistry at the University of Colorado at Boulder in 1941. Shortly thereafter, he became a Chemistry instructor at the University of Idaho and then in 1943, returned to the University of Colorado in Boulder for a Ph.D. in Chemistry with a minor in Microbiology. After two years as a research chemist at the Battelle Memorial Institute in Columbus, Ohio, Dr. Castle accepted a position at the University of New Mexico as an Assistant Professor of Chemistry. He served as Chairman of the Chemistry Department from 1963 until 1970 before moving to Brigham Young University as Professor of Chemistry.

In 1981, Dr. Castle joined the faculty at University of South Florida as a Distinguished Research Professor. He and his wife, Ada, were a vibrant part of the Chemistry Department and for many years sponsored the Castle Lecture Series, which brought in numerous prominent scientists for lectures at USF .

A prolific researcher, Dr. Castle was an internationally recognized father figure in heterocyclic chemistry, both for his research and his involvement in meetings, symposia, and editorial boards. In 1964, he founded the Journal of Heterocyclic Chemistry and served as its editor. He also edited the Lectures in Heterocyclic Chemistry series, a publication of plenary lectures given at the International Congresses of Heterocyclic Chemistry and was the American advisory editor for the English translation of the Russian Journal of Heterocyclic Compounds. He lectured at hundreds of institutions worldwide. He was General Chairman of the First International Congress of Heterocyclic Chemistry held in Albuquerque (1967), Secretary of the Second International Congress held in Montpellier, France (1969), and Vice-President of subsequent Congresses held in Sendai, Japan, Salt Lake City, Utah, Ljubljana, Yugoslavia, and Tehran, Iran. Dr. Castle was also Chairman and Committee Member for the American Chemical Society. In addition, he was cofounder of the International Society of Heterocyclic Chemistry, which he served as Chairman of the Executive Committee, and President (1973-1975). Professor Castle received numerous awards and honors, including the prestigious International Award in Heterocyclic Chemistry (1983) for outstanding contributions to the field of heterocyclic chemistry, presented in Tokyo, Japan. Dr. Castle was listed in the first edition of Who's Who in Science and in Who's Who in the World.

The Chemistry Department remains deeply indebted to Professor Castle for his many outstanding contributions to the Department, and to science overall. He would have been a strong supporter of this student symposium, and thus, it is fitting that we dedicate this and future symposia to his memory.

Special Thanks

Dr. Dean F. Martin is Distinguished University Professor Emeritus and Director of the Institute for Environmental Studies at the University of South Florida, where he has been a member of the faculty since 1964. Dr. Martin received his B.A., with Honors, from Grinnell College (1955), where he met his future wife Barbara while both were chemistry majors. They were married in 1956 while both attending Pennsylvania State University as graduate students and in 1958 Dr. Martin received his Ph.D and Mrs. Martin her Master's degree. In 1958-59, he was a National Science Foundation Post-Doctoral Fellow at University College, London after which he returned to the States and accepted a faculty position at the University of Illinois, Urbana-Champaign, as Instructor and Assistant Professor of Inorganic Chemistry (1959-1964). He received (1969-1974) a Career Development Award from the Division of General Medical Sciences, NIH, to study the chemistry and chemical environment of algal toxins. In 1970-71, he was a Visiting Professor of Physiology and Pharmacology at Duke University Medical Center.

Dr. Martin and his wife share research interests concerned with coordination chemistry in natural water systems, including problems of red tide and aquatic weeds. Currently, they are investigating the removal of metals and organic compounds from water by means of supported chelating agents. Dean Martin is the author or co-author of over 300 publications, including four books. He was the recipient of the 1975 Florida Award and the 1987 Civic Service Award of the Florida Section, ACS; in 1978, he received the F. J. Zimmermann Award in Environmental Science from the Central Wisconsin Section, sponsored by Zimpro Inc.; and in 1983, he was elected Fellow of the American Association for the Advancement of Science. Dean and Barbara Martin were the co- recipients of the 1994 Medalist Award of the Florida Academy of Sciences, its highest award. Dean Martin has been active in the Florida Section of the American Chemical Society (Chairman, 1986), and he has held several positions in the Aquatic Plant Management Society (President, 1986-87). Both of the Martins have received the Alumni Award of Grinnell College.

The Martins have endowed six chemistry funds, including the George Bursa Award, given annually to a deserving graduate student within the Chemistry Department who has demonstrated notable professional dedication and consideration for others, as well as a Graduate Student Travel Award. Together the Martins have edited Florida Scientist since January 1984 and are now Editors Emeriti. Dr. Martin initiated and continues to edit the departmental newsletter and has written a departmental history to coincide with the 40th Anniversary of the founding of the department.

The Martins have six children; Diane, Bruce, John, Paul, Brian, and Eric, and seven grandchildren.

Plenary Speaker, Sherri A McFarland Ph.D.

Professor Sherri A. McFarland earned a BA in Chemistry from Hendrix College in 1996 (mentor: Prof. Tom Goodwin) and a PhD in Chemistry from the University of California San Diego in 2003 (mentor: Prof. Nat Finney). Her PhD thesis involved the preparation and photophysical characterization of organic and inorganic compounds as luminescent chemosensors for ion and molecule recognition. Prof. McFarland then moved to Canada and completed a postdoctoral fellowship at Dalhousie University (2003-2005) with Profs. Norm Schepp and Fran Cozens where she used femtosecond laser spectroscopy to study the ultrafast photophysical dynamics of transition metal complexes. Professor McFarland started her independent career at Acadia University, a primarily undergraduate university in Canada. While at Acadia, she established a multidisciplinary cancer research program in the area of photomedicine, working closely with undergraduates, MSc students, and research staff. In 2011, she partnered with Theralase Technologies, Inc. to develop photodynamic compounds for treating cancer with PDT and in 2012, she co-founded (with Dr. Colin Cameron) a biotech start-up PhotoDynamic, Inc. to commercialize a photoactive antimicrobial natural product extract for dentistry. In 2016, Professor McFarland and her research group relocated to the US, where they continue to be heavily involved in translational research that has resulted in 4 human clinical trials to date (3 completed, 1 underway).

Plenary Presentation

Light-triggered Metallodrugs for Cancer Therapy

Photomedicine is an interdisciplinary field where chemistry and light meet to fight disease. Photodynamic therapy (PDT) is a special branch of photomedicine that employs a photosensitizer, light, and oxygen to destroy cancer cells with spatiotemporal selectivity. The photosensitizers used for PDT have historically been organic molecules, specifically porphyrins and other tetrapyrrole-related structures. Given the important role of metals in medicine, metallated analogs of these traditional systems (as well as metal complexes of markedly different architectures) have attracted considerable attention in recent years. Our TLD1433 (Ruvidar®), a metal complex designed in our laboratory, is an example that is also the first ruthenium-based photosensitizer for PDT to advance to human clinical trials. This seminar will discuss the design and development of TLD1433 for treating bladder cancer with PDT and share some of our current research directions.

Morning Oral Sessions

Oral Session A (CHE 303)

Rama Mahita Kambhampati	09:30am - 09:50am
Alissa “Brooke” Anderson	09:50am - 10:10am
Thomas Egan	10:10am - 10:30am
Bhanu Sharma	10:30am - 10:50am

Oral Session B (CHE 217)

Simeon Fagbodun	09:50am - 10:10am
McKenna Parker	10:10am - 10:30am
Samuel Camilli	10:30am - 10:50am

Oral Session C (CHE 302)

Shelby Kell	09:50am - 10:10am
Yu Yu Win	10:10am - 10:30am
Lubem Agbendeh	10:30am - 10:50am

Afternoon Oral Sessions

Oral Session D (CHE 100)

Yafeng Wang	01:00pm - 01:20pm
Stine Sofie Olsen	01:20pm - 01:40pm
Sylvester Osei Bobbie	01:40pm - 02:00pm
intermission	02:00pm - 02:10pm
Alexander Mariscal	02:10pm - 02:30pm
Nathaniel Schmidt	02:30pm - 02:50pm

Oral Session E (CHE 111)

Rachel Weiss Clark	01:00pm - 01:20pm
Emmanuel Eni	01:20pm - 01:40pm
Sang Phan	01:40pm - 02:00pm
intermission	02:00pm - 02:10pm
Qaisar Maqbool	02:10pm - 02:30pm
Guy W. Dayhoff II	02:30pm - 02:50pm

Oral Presentation Abstracts (Morning - Session A)

Innovations in Managing Geosmin and 2-Methylisoborneol in Water Systems and Aquaculture: Detection and Mitigation Strategies

Geosmin and 2-methylisoborneol (2-MIB) are secondary metabolites produced by various organisms, introducing undesirable flavors to public water supplies, aquaculture, and various products. Ongoing research delves into unraveling the factors influencing their expression and crafting effective mitigation strategies, demanding precise detection methods. While 2-MIB is commonly linked with a muddy aroma, Geosmin imparts a scent reminiscent of old books or must. These naturally occurring compounds are generated by cyanobacteria, actinomycetes, fungi, and bacteria in diverse environments.While these pose no direct hazard, their presence may signal the existence of other hazardous substances produced by the same organisms. This study aims to delve into the latest advancements in detecting and mitigating geosmin and 2-MIB, shedding light on the intricacies of their expression, the difficulties in differentiation, and the broader implications for water systems and aquaculture.

Presented by: Rama Mahita Kambhampati *(Graduate, Analytical Chemistry)*

Understanding the Role of Metal Halide Semiconductors as Photosensitizers for the Inhibition of Target Bacteria and Fungi

The escalating threat of antimicrobial resistance poses a significant global health challenge, demanding innovative solutions. Hybrid organic-inorganic metal halide semiconductors are highly versatile materials with applications in numerous fields resulting from their unique optoelectronic properties, which can be tailored to elicit an optimal photoresponse for effective antimicrobial interventions. We synthesized several biocompatible phosphine metal halides with intrinsic water stability, alongside optimal optoelectronic properties and potential for use as inhibitory agents. These compounds exhibit excellent optical properties, with broad, band edge emission and have been determined to be Type I ROS generators. Evaluation of their inhibitory activity against diverse target bacteria and fungi enhances our understanding of their role as biological agents.

Presented by: Alissa "Brooke" Anderson *(Graduate, Inorganic Chemistry)*

Investigating the thermal stability of anisotropic metal nanoparticles on a TiO2 support

In the field of catalyst design, it is a common strategy to decorate metal nanoparticles (NPs) onto support materials to enhance their catalytic performance and stability. During the preparation of these composite materials, annealing at elevated temperatures is a required step for activation. While fine metal NPs are typically grown directly on the support, shape-controlled metal NPs are almost exclusively synthesized colloidally and must be immobilized on the support surface. During annealing, metal NPs are known to significantly change shape due to their unstable surface facets, diminishing their catalytic activity. Therefore, it is necessary to find ways to

preserve their shape through the catalyst preparation process. Here, we investigate the shape stability of anisotropic Au NPs on a TiO2 support. By depositing thin shells of different metals (Ag, Pd, Pt), we find that their shape stability can be altered and even enhanced, while imparting improved intrinsic catalytic activity.

Presented by: Thomas Egan *(Graduate, Inorganic Chemistry)*

Revisiting the seed-mediated growth of core-shell nanoparticles: localizing the reducing agent on the seed surface

Core-shell nanoparticles' physical and chemical properties are highly dependent on the choice of the material and have shown great potential in catalytic, biosensing, photothermal, surface-enhanced Raman spectroscopy (SERS), and drug delivery applications. These nanostructures are generally synthesized by a seed-mediated approach where core nanoparticles are used as seeds, and shell metal precursor is deposited on it in the presence of a reducing agent. This approach has two main drawbacks. The first is the uncontrollable self-nucleation of shell metal, which is usually solved by the slow injection of the precursor into the solution and the second drawback is the spontaneous galvanic replacement which limits the synthesis of the core-shell nanostructure. To counter these drawbacks, our idea is to localize dopamine (DA) as a reducing agent on the surface of the core nanoparticle. Briefly, Poly-Dopamine can prevent act as a stabilizer for core metal nanoparticles and reduce metal salts.

Presented by: Bhanu Sharma *(Graduate, Inorganic Chemistry)*

Oral Presentation Abstracts (Morning - Session B)

Release efficiency of liposomes-encapsulated proteins via SAW

Liposomes are synthetic, spherical lipid vesicles with a lipid bilayer composed of hydrophilic head regions and a hydrophobic tail region, with an aqueous core. Due to their size and cargo customizability, they are ideal drug delivery candidates. Detergents such as sodium dodecyl sulfate (SDS) are commonly used to disrupt lipid membranes and release encapsulated cargo. However, detergents can affect the integrity of the cargo, and their efficacy varies depending on bilayer composition. This project aims to determine the release efficiency of liposome-encapsulated low molecular weight proteins via disruption using surface acoustic waves (SAWs). Liposomes are subjected to various SAW frequencies and timeframes to initiate cargo release. Surface acoustic wave nebulization (SAWN) coupled with corona discharge (CD) ionization is used to ionize the disrupted samples for analysis via Ultraviolet-Visible (UV-Vis) Spectroscopy.

Presented by: Simeon Fagbodun *(Undergraduate, Analytical Chemistry)*

Interaction of bacterial effector proteins with host cell chaperones

Pathogenic bacteria utilizes effector kinase proteins to manipulate cellular pathways and promote an environment conducive to survival and propagation by inhibiting the immune defense of the host cell. In this project, we focus on bacterial effector proteins that lead to the inhibition of the NF-kB (nuclear factor kappa-light-chain-enhancer of activated B cells) pathway, which regulates the inflammatory response within the cell. Understanding how bacterial effector proteins function requires a detailed understanding of the pathways of recruitment for substrates in the host cell, the targets within the host cell, and how the protein interacts with host cell proteins. In this project, we study how effector kinase proteins interact with chaperone proteins found in host cells. Understanding the mechanisms of the bacterial effector kinase can lead to the development of more effective antibiotic treatment and increased intervention options for the bacteria that utilize effector proteins.

Presented by: McKenna Parker *(Undergraduate, Biochemistry)*

Infinite Insights: A Journey of Student-Led Tutoring Excellence

Since its inception in Fall 2020, the USF Chemistry's Tutoring Society has helped thousands of students across a variety of undergraduate courses. Among these are General Chemistry I & II, Organic Chemistry I & II, Inorganic Chemistry, Analytical Chemistry, and more. The tutoring lab has been vastly successful for two reasons: 1) it is set up using peer-to-peer instruction and 2) utilizes Microsoft Teams for large-scale accessibility. The mean number of tutors per semester since Fall 2020 is 44. The most interesting finding is that the ratio of hours per tutor has nearly tripled from Fall 2020 (7.27 hours/tutor) to Fall 2023 (21.60 hours/tutor). With this increased demand on our tutors, this presentation will discuss our plans for the coming semesters which includes 1) establishing a comprehensive Canvas course filled with resources, 2) increased marketing and outreach, and 3) partnerships with other student organizations.

Presented by: Samuel Camilli *(Undergraduate, Chemistry Education)*

Oral Presentation Abstracts (Morning - Session C)

Design of a photoswitchable ligand as a JAK2 inhibitor

Photopharmacology is an emerging field that uses the power of light for the precise modulation of drug activity. Through directed light, a photoswitchable ligand may be activated, or deactivated, which provides a level of control over the biological activity of molecules. The development of drug analogues, designed to incorporate a photoswitchable segment within a ligand, holds the promise of creating controllable and selective inhibitors. As molecular photoswitches undergo light-induced isomerization associated with a large geometrical transformation of the molecule, the introduction of a photoswitch into a ligand would allow for spatiotemporal control. The conformational change of the photoswitch results in an augmented binding affinity for one isomer and a diminished affinity for the other isomer. The active isomer works as a potent inhibitor which effectively disrupts the targeted protein and interrupts downstream signaling pathways.

Presented by: Shelby Kell *(Graduate, Biochemistry)*

Rational design and synthesis of α-helix-mimicking sulfonyl-γ-AApeptide sequences for disrupting cMyb-Kix interaction

cMyb, a transcription factor, involves in proliferation, survival, and differentiation of hematopoetic cells by interacting with KIX domain of CREB-binding protein. However, overexpression of cMyb causes leukemia, breast and colon cancers. We designed stapled 1:1 α/Sulfonyl-γ-AA hybrid peptides and homogeneous Sulfonyl-γ-AA sequences to mimic cMyb binding interface. Preliminary studies including the binding assay, NMR study and cell permeability were performed. Our peptidomimetics showed much enhanced binding affinity, larger chemical shift and better permeability compared with wild type cMyb.

Presented by: Yu Yu Win *(Graduate, Biochemistry)*

Immunogenicity and Efficacy of Cell Wall Proteins: Potential Vaccines for Clostridioides difficile Infection.

Clostridioides difficile infection (CDI) is the primary cause of pseudomembranous colitis, particularly in healthcare settings due to antibiotic-associated diarrhea. The main risk factor is the ingestion of spores activated by broad-spectrum antibiotics, disrupting the gut microbiota. The bacteria resist the host immune system, leading to colonization and mucosal adhesion. This study focused on three cell wall proteins (Cwp18, Cwp19, and Q181Y8) from the hypervirulent C. difficile strain R20291, involved in bacterial autolysis. These proteins were expressed in Escherichia coli, purified, and tested for immunogenicity and efficacy in a mouse model. Initial results indicate enhanced protective immunity, suggesting potential as vaccine candidates against CDI. Ongoing studies aim to confirm the efficacy of these proteins as alternative vaccines.

Presented by: Lubem Agbendeh *(Graduate, Biochemistry)*

Oral Presentation Abstracts (Afternoon - Session D)

RET protac for targeting abberant RET protein degradation.

Every year, about 1%-2% non-small cell lung cancer(NSCLC) are induced by RET abberant expression. Until now, no protac compound has been developed to degrade RET protein. Here, we design a series of protac molecules using different E3 ligands and linkers. The lead compound, YW-D-21-4, not only show good RET protein degradation ratio and inhibition activity, but also have good PK data in animal test. With further optimization, YW-D-21-4 analogues could be developed into the first effective RET degrader to kill abberant RET expression tumors.

Presented by: Yafeng Wang *(Graduate, Organic Chemistry)*

Isolation and structure elucidation of new sesquiterpenes from the Irish deep-sea coral Anthothela grandiflora

Natural products have been used as medicine to treat humans since ancient times due to their secondary metabolites showing promising therapeutic properties. Today, 60% of marketed drugs are direct natural products or natural products derived, 2% being from the deep-water ecosystem. Lack of light, low levels of oxygen, and intense pressures in the deep-sea contribute to modifications of the organism's primary and secondary metabolites, creating chemical compounds not found in shallow-water organisms. This research explores the chemistry found in the deep-sea coral Anthothela grandiflora, resulting in 16 new cadinene-like sesquiterpenes. The terpenes were isolated by VLC followed by repeated rounds of purification using RP-HPLC. NMR experiments were used for structure elucidation and determination of relative stereochemistry, while experimental and calculated ECD spectra, DP4+ predictions, and x-ray crystallography were used to determine the absolute configuration of the compounds.

Presented by: Stine Sofie Olsen *(Graduate, Organic Chemistry)*

New Natural Products from Deep Sea Coral Antipathes

The ocean is a diverse pharmacological environment which inhabits mostly corals, tunicates and sponges. Antipathes is a genus of corals in the order Antipatharia, composed of black coral is known to produce therapeutic class of compounds such as alkaloids, terpenoids, sphingolipids and steroids. This research project seeks to generate novel compounds from the coral Antipathes. Extracts will be concurrently subjected to bioassay and nuclear magnetic resonance (NMR) spectroscopy guided approaches to aid in the search for novel compounds with biological activity.

Presented by: Sylvester Osei Bobbie *(Graduate, Organic Chemistry)*

Charge Assisted Recognition in Water by Cationic Host Exhibiting Preference for Kosmotrophes

Anion recognition in aqueous solution is difficult due to strong solvation of anions by water, more so than for analogous cations. Reported supramolecular hosts working in 100% water often exhibit a preference for weakly solvated anions due to this. To achieve selectivity for strongly solvated anions according to the Hofmeister series, we have synthesized a macrocyclic host with +2 charge which binds -2 anions with millimolar affinity in 100% water. Our molecule was designed to have a preorganized structure with amide N-H bonds and electron-deficient para-pyridinium C-H bonds pointing into the binding cavity as hydrogen bond donor groups. We reason that the +2 charge resulting from pyridine alkylation helps to electrostatically attract anions while also inductively strengthening hydrogen bond donor groups. Binding studies with a synthesized control molecule with an analogous structure but no cationic charge illustrate the importance of this design feature.

Presented by: Alexander Mariscal *(Graduate, Organic Chemistry)*

Total Synthesis of Friomaramide

Friomaramide is a modified linear hexapeptide isolated from the Antarctic sponge Inflatella coelosphaeroides. It is potently bioactive against Plasmodium falciparum, inhibiting greater than 90% of liver-stage development at a concentration of 6.1μM. The C-terminus of Friomaramide is structurally unusual, consisting of a Z-configured indolic enamide. Our synthesis takes a convergent approach, separately building the N-methylated peptide and indolic enamide moieties, and finally coupling to yield the natural product.

Presented by: Nathaniel Schmidt *(Graduate, Organic Chemistry)*

Oral Presentation Abstracts (Afternoon - Session E)

Mechanistic insights into ligand-to-metal charge transfer photocatalysts from ultrafast spectroscopy

Pharmaceutical synthesis relies on catalytic processes for cost-effective preparation of a wide variety of pharmacophores at scale. One major drawback of these synthetic methods is the requirement of high reaction temperatures and caustic reagents. Ligand-to-metal charge transfer (LMCT) photocatalysts represent a promising alternative as they can achieve thermodynamically onerous reactions under mild conditions and have demonstrated a range of catalytic reactivity spanning from selective C-H bond activation to cross-coupling. This reactivity along with fruitful product yields from these comparatively benign first row transition metal complexes has garnered significant attention for LMCT photocatalysis; however, LMCT photocatalysis has been plagued by unexplainably low per photon efficiencies, necessitating long irradiation times to furnish complete product conversion. This has stirred up demand for reliable mechanistic insight into the LMCT excited state, which has been largely elusive

Presented by: Rachel Weiss Clark *(Graduate, Physical Chemistry)*

Elucidation of Structural Parameters in O-6-methylguanine Containing DNA Sequences Which May Determine Repair Enzyme Recognition through MD Simulation

The base excision repair pathway begins with the recognition and excision of non-helix-distorting DNA lesions by DNA glycosylase enzymes. The enzyme action often involves base flipping. Efficiency depends on the local sequence context. Here we aim to detail the structural determinants of enzyme lesion recognition and excision, by exploring the structural impact of the O-6-methylguanine (O6MeG) lesion via molecular dynamics simulations. Key findings demonstrate that DNA sequences containing O6MeG exhibit lower persistence lengths than control sequences, suggesting that DNA deformability facilitates repair. Principal component analysis revealed significant structural differences between damaged and undamaged DNA is primarily due to the ribose sugar puckering. The sugar moiety puckering in O6MeG containing DNA not only increases their flexibility but also allows access to a wider conformational space inaccessible by the control sequences. This might be the basis of lesion recognition.

Presented by: Emmanuel Eni *(Graduate, Physical Chemistry)*

Computational study of Mad2 wildtype and its mutants

Cells employ a series of cell cycle checkpoints to ensure a proper cell division. One such cell cycle checkpoint, known as the spindle checkpoint, occurs during the transition from metaphase to anaphase. The essential spindle checkpoint protein Mad2, mitotic arrest deficient 2, delays the transition via a conformational change from its inactive open state to its active closed state. Mutants of Mad2 blocked this crucial transition by locking Mad2 into a single conformation. To

gain insight into the effect of each mutant, we performed 2 μs of unrestrained MD simulations of wild and mutant variants of Mad2. By using a series of analysis such as RMSD, covariance, quasi-harmonic modes, we aimed to find common patterns among the mutants. Additionally, analysis of hot spot residues will reveal similar trends that can explain the dynamic behavior of Mad2 mutants.

Presented by: Sang Phan *(Graduate, Physical Chemistry)*

Photophysical comparison between Tetra-N-Methyl-Pyridyl Porphyrin (TMPyP) and Meso-tetra(4-N,N,N-trimethylanilinium) porphyrin (4TANP)

Porphyrins are a diverse class of tetrapyrrole macrocyles that have wide ranging applications in light harvesting, chemical sensing, and catalysis. The electronic structure of the porphyrin macrocycle modulates the chemical properties. In general, excitation of tetraphenyl based porphyrins (TPPs) leads to population of a singlet S2 state that rapidly decays to a lower energy singlet S1 state through vibrational relaxation processes. The 1S1 state decays via radiative and non-radiative relaxation as well as inter-system crossing to a 3T1 state. In contrast, the excited state of the TMPyP porphyrin had a charge transfer (CT) state that mixes with the 1S1 and is due to the positive charges associated with the pyridinium rings. The extent of mixing between the CT and S1 states are affected by solvent polarity and the orientation of the pyridinium groups relative to the porphyrin plane. Here, the excited state photophysics of 4TANP, are examined to probe for the presence of similar CT state.

Presented by: Qaisar Maqbool *(Graduate, Physical Chemistry)*

Machine Learning Velocities to Propagate Molecular Dynamics Simulations

Time evolution in molecular dynamics (MD) simulations requires knowledge of velocity changes. These are obtained from partial derivatives of potential energy. In principle, high accuracies can be achieved when potential energy derivatives are estimated from electronic structure theory. However, such treatments are computationally inefficient and limit application to small systems. Numerous efforts are in place to explore the capability of machine learned potential energy functions to improve efficiency while maintaining accuracy. Here we propose an alternative strategy wherein velocities themselves are machine learned and predicted. We focus on ten isolated harmonic oscillators differing in masses and bond coefficients: H2, N2, O2, F2, Cl2, Br2, I2, HCl, HBr, and NO. We report that long-short-term memory networks (LSTMs) can indeed be trained on a particle's historical velocities to predict velocity updates with 99.9% accuracy. We also show that they can be used to propagate MD conserving both kinetic and potential energies.

Presented by: Guy W. Dayhoff II *(Graduate, Physical Chemistry)*

Poster Presentation Abstracts (Midday - Posters)

An educational experiment in the use of gas chromatography

Here I present an experiment for providing instruction as to the operation of a gas chromatograph and subsequent analysis. The aim of the experiment is to determine the caffeine content in a sample of store-bought coffee through the use of gas chromatography. The experiment uses internal standard addition of adenine. We hope to be able to use this method to instruct students as to the operation of a gas chromatograph, sample preparation, data analysis, and the use of the internal standard method.

Presented by: Ilya Bulanov *(Undergraduate, Analytical Chemistry)*

Dietary Reconstruction from Stable Isotopic Analysis: An Case Study from Medieval Transylvania

This study aims to use bulk stable isotope analysis of carbon (13C) and nitrogen (15N) to reconstruct diets in bioarchaeology, focusing on medieval peoples from Transylvania. The bone samples were excavated from the Papdomb archaeological site in eastern Transylvania, now central Romania. Collagen was extracted from the samples by demineralizing and solubilizing the bone, then freeze-dried. For the bulk stable isotope analysis, samples were analyzed by Continuous Flow Elemental Analyzer Isotope Ratio Mass Spectrometry (CF-EA-IRMS), and the composition reported in per mil notation. Analysis of the isotopic composition allows for a general reconstruction of diet based on the isotopic ratios of photosynthetic pathways.

Presented by: Dorothea Fennell *(Undergraduate, Analytical Chemistry)*

Method Development for Isolation of Atmospheric Microplastics from Rainwater

Atmospheric microplastic (MP) pollution is an increasingly growing field of research. Current data suggests long-distance atmospheric transport of MPs. Sample processing is not yet standardized, and methods strongly depend on research objectives. The aim of this project is to validate current methods for use with bulk MP deposition in rainwater. Methods for volume reduction, organic digestion, and density separation were evaluated for recovery rate and polymer integrity. This study utilized μRaman spectroscopy and particle analysis via digital imaging to investigate the efficacy of these methods. Procedures were evaluated by Raman spectra matching-degree, processing duration, and reagent usage to assess the suitability for frequently used methods in MP research. Functionality was assessed regarding observable matrix interferences and the data quality achieved. The methods developed herein will be applied to environmental samples to explore spatial patterns of MP pollution in Tampa Bay.

Presented by: Braden Foerch *(Undergraduate, Analytical Chemistry)*

Determining the Alcohol Content in Hand Sanitizer Gels

Hand sanitizer gel is widely used across the country, especially after the outbreak of the infamous Coronavirus. Moreover, with flu season on the rise, hand sanitizers are continuously being made and put on the market. However, before it goes on the market, the alcohol content needs to be quantified and verified to comply with the industry standards set by regulatory agencies to ensure the alcohol content matches the amount in the bottle. Therefore, the project will quantify the alcohol content in various hand sanitizers using gas chromatography. The method that will be used in this experiment is cataloged by the United States Pharmacopeia to analyze ethanol concentrations. A Flame Ionization Detector and the SH-Rtx-624 capillary column will be used for this method.

Presented by: Brianna Nazario *(Undergraduate, Analytical Chemistry)*

Acoustic Disruption for use in Dye Incorporation of Lipid Vesicles

Exosomes are nanosized extracellular vesicles that play a crucial role in intercellular communication. Due to their similar structure to cell membranes, researchers began studying their use as carriers for drug delivery, which led to the development of liposomes, a self-assembled vesicle that consists of a lipid bilayer and aqueous core. Their versatile composition makes them an excellent choice in drug delivery and standards for studying exosomes. Liposomes and exosomes can be used for tracking in biological systems through the incorporation of dye. The use of surface acoustic waves (SAWs) may be employed for liposome dye incorporation. To facilitate this technique, liposomes and dye will be placed on a SAW chip to induce lysis for a duration of 0-30 seconds at different frequencies. After lysis, separation and analysis of the dye and liposomes will be conducted using high performance liquid chromatography (HPLC) with size exclusion chromatography (SEC) and fluorescence microscopy.

Presented by: Autumn Nielsen *(Undergraduate, Analytical Chemistry)*

Using MATLAB to Process and Model Time-Dependent Spectroscopy Data

Chemical kinetics relies upon experimental data regarding the change rates of a reaction in order to better understand the mechanisms between chemical species involved. Using MATLAB, I am seeking to write a program that can process imported time-dependent spectroscopic data, determining a model of reaction rate. If successful, rate law information could be determined from simply importing data from the system, making a simple tool for chemists looking to quickly ascertain information on a reaction mechanism.

Presented by: Andrew Reid *(Undergraduate, Analytical Chemistry)*

Analysis of high-frequency vibration-induced microvesicle disruption

Microvesicles are biological 0.1-1.0 μm sized hollow spheres made of a lipid bilayer that carries biological material such as RNA and proteins. Due to these properties, they pose as an ideal candidate for localized drug delivery and as a tool for diagnosing diseases such as cancer. Using

high-frequency vibrations, microvesicles can be disrupted releasing the contents within them providing important information on biological processes taking place within an organism. To better understand the microvesicle disruption a combination of analytical techniques which include UV-Vis, Size exclusion chromatography, Scanning electron microscope, and Dynamic light scattering were used to get a qualitative idea of the disruption caused at high-frequencies over 10MHz.

Presented by: Harrison Ryczek *(Undergraduate, Analytical Chemistry)*

Non-contact Electrostatic Sampling of Compounds for MS/MS Analysis

The Fun Fly Stick (FFS) is used to add an electrostatic potential to the tip of the instrument to aid in the collection of the compounds when in close proximity to the sample. There is no need for physical contact to occur between the FFS and the bag with the compound on it, as the electrostatic field generated is strong enough to extract and hold onto the particles until they are analyzed. The analysis process is done through careful collection of the sample and then performing tandem mass spectrometry (MSMS) on the sample with the LTQ Ion Trap Mass Spectrometer. The results are then compared with those of the expected MSMS library spectra for the known compound/drug sampled. The purpose of utilizing this method is to aid in the prevention of cross-contamination and interference in data collection in a typical forensic science field. This method is used to extract the drug sample without touching, swabbing, or otherwise interfering with the other possible layers of evidence.

Presented by: Mackenzie Sampson *(Undergraduate, Analytical Chemistry)*

Investigation of the Potential Impact of Lyophilization on Exosomes and Size

Liposomes are nano-sized, spherical vesicles containing a phospholipid bilayer. These vesicles can be easily synthesized and customized and are essential in the medical field as drug-delivery vehicles. Understanding the versatility of liposomes will produce a standard to be applied to more complex structures such as exosomes. Exosomes are extracellular vesicles (EVs) with a diverse functionality profile of carrying information and various cargo and can be used as biomarkers. Analyzing these lipid vesicles can come with hurdles, including maintaining stability and preventing aggregation. A potential solution to this is applying the process of lyophilization, a process that extracts H2O from a product after freezing and placing it under a vacuum, allowing the product to convert directly from a solid to vapor. Thus, an investigation of the effect on the size of liposomes will occur by using dynamic light scattering (DLS) before and after lyophilization with and without a cryoprotectant.

Presented by: Philrosen Luchy Monfiston Sejour *(Undergraduate, Analytical Chemistry)*

Anticancer Agents and Peptidomimetics: Pharmacological Biosynthesis

Numerous physiological and pathological stimuli induce programmed cell death, and the Bcl-2 family of oncoproteins plays a central role in this regulation. Uncontrolled cell survival due to

Bcl-2 overexpression has been proven to make a significant contribution to tumor formation. With this in mind, we have directed our attention toward the synthesis of a variety of non-peptide inhibitors of oncoproteins Bcl-2. Recently, we have disclosed efficient protocols leading to the synthesis of carbamate, polyamine, azadepsipeptide, and dithiocarbamate peptidomimetics, respectively. This study is now being extended to the synthesis of other de novo analogs with similar structural features to natural proteins, that may interrupt protein-protein interactions and furthermore, may serve as potential therapeutics in clinical chemotherapy. Utilizing our aforementioned protocols, our research is now being employed for the synthesis of other interesting novel artificial biomolecules.

Presented by: Abigail Baker *(Undergraduate, Biochemistry)*

The Biosorption of Copper Using Dried Fruits

Copper runoff from farming and manufacturing can contaminate drinking water, leading to severe health problems. To develop an accessible method for people to purify copper from water, this research explored the potential for dried fruits' cellulose to bind with copper ions through biosorption. After graphing a calibration curve for the copper sulfate solution, each trial's copper solution experienced biosorption with dried dates, dried apricots, raisins, dried cranberries, or dried cherries, where each dried fruit contained different cellulose composition. Then, a colorimeter measured each copper solution's absorbance, which allowed their final concentrations to be calculated. The experiment found a positive correlation between dried fruits' cellulose composition and the biosorption of copper ions. Namely, dried dates had both the highest cellulose concentration and the most significant decrease in copper concentration. Hence, dried fruits hold potential for copper's biosorption.

Presented by: Roy Chen *(Undergraduate, Biochemistry)*

Novel Covalent Inhibitor Targeting RET kinase

REarranged during Transfection(RET) is a receptor tyrosine kinase which is a crucial factor in the normal development and maturation of various tissues. Genomic alterations in RET kinase, including fusions and activating point mutations, result in overactive RET signaling and unregulated cell growth. Cancers with RET fusions and RET-mutant medullary thyroid cancer(MTC) heavily rely on this activated kinase for their proliferation and survival. This dependence makes such tumors highly responsive to small molecule inhibitors targeting RET. We recently discovered an intriguing compound capable of forming a covalent bond with the cysteine in the RET protein(G810C), thus acting as a covalent inhibitor. This inhibitor efficiently blocks the kinase, leading to the inhibition of cancer cell growth. We performed functional group modifications on this lead compound to investigate the binding capabilities of analogs with RET.

Presented by: Yunpeng Cui *(Graduate, Biochemistry)*

Validation of SETDB2 protein expression in SETDB2 cell-specific knockouts

Gene expression control is vital to regulate cellular activity and responses. Histone methylation alters the chemical interactions between histone complexes, DNA, and other proteins and is one way that gene expression is controlled. SETDB2 is a H3K9 methyltransferase that is highly associated with the proinflammatory response and plays a key role in liver metabolism. The Osborne lab investigates the mechanism of SETDB2 as a regulator of gene expression for metabolic and immune systems. SETDB2 is both promoted under metabolic stressors and associated with metabolic and inflammatory diseases. Therefore, we hypothesize that SETDB2 deficiency will have protective effects against immuno-metabolic disease phenotypes. Detection of SETDB2 via immunoblot is essential to confirm the cell specific knockout of SETDB2 in mice. The goal of this project is to optimize immunoblot conditions for SETDB2 detection in mouse hepatocytes and bone marrow macrophages.

Presented by: Annabelle Elsner *(Undergraduate, Biochemistry)*

The Kinetics of PAL

Peptidylglycine alpha-amidating monooxygenase, or PAM, is a critical enzyme in the body that has two parts to its reaction: One known as PHM, and the other PAL. Both of these can be examined through a number of different laboratory experiments, which can test the conditions and compounds that allow for this enzyme to function in the body. The research conducted in this project focuses on a preliminary investigation into the PAL portion of this enzymatic reaction. More specifically, it is important to understand the kinetics of this enzyme, and so in a series of experiments demonstrated in this research both potential substrates and inhibitors are tested with varying degrees of success. The glyoxylate assay procedure is the foundation upon which most of the physical lab work is built of off. By the end of the project, the goal is to have at least a more formative idea of the types of substrates which work well with PAL and the enzyme's potential inhibitors.

Presented by: Collin Greenhalgh *(Undergraduate, Biochemistry)*

Proteomic Profiling of Tribolium castaneum via Stearoyl and Oleoyl Fatty Acid Amide Probes

The role of Fatty Acid Amides (FAAs) in biological processes has only been explored on a small scale, yet their presence in a wide variety of organisms indicate there is more to be discovered. My research involves the interaction between various fatty acid analogs and the model proteome of Tribolium castaneum using a process known as Binding-Based Proteomic Profiling (BBPP). Stearoyl and Oleoyl fatty acid amides are functionalized with diazirine groups, allowing for strong covalent bonding between probe and the target proteins upon UV exposure. Alkyne groups on the fatty acid probes allow for tagging with either biotin or a fluorescent dye through a click reaction. Tagged proteins can then visualized or be isolated via an avidin column, allowing for specific isolation of proteins interacting with the probes. Enriched protein samples are analyzed through LC-MS for characterization and comparison to orthologs in other species.

Presented by: Patrick Jessup *(Undergraduate, Biochemistry)*

What Is the Effect of a Mixed Culture of Pseudomonas fluorescens and Anabaena on the Degradation of Polyvinyl chloride?

As our use of plastics continues to increase, the difficulty in degrading these plastics when they reach natural waterways increases as well. The degradation of polyvinyl chloride plastic (PVC) in particular, has posed difficulties for researchers as PVC's alipathic structure complicates the degradation process. The objective of this study was to expose two bacteria - Pseudomonas fluorescens and Anabaena - to each other to utilize a combination of the biochemical processes of both specimens to degrade this plastic. To test this, samples of PVC cloth were massed before and after exposure to these two samples of bacteria to determine if degradation was present or not. After undergoing thesetrials, the methodology demonstrated that the proposal to expose both bacteria to each other to attempt to degrade PVC was a success, as the degradation rates of this combination of bacteria surpassed previous degradation rates of PVC in the field.

Presented by: Ojas Kalia *(Undergraduate, Biochemistry)*

Combinatorial library synthesis by using γ-AA cyclic peptides against protein targets

Combinatorial library synthesis is a powerful approach in chemistry and molecular biology, enabling the rapid generation of diverse molecular structures for drug discovery or materials science. This method involves the systematic combination of building blocks and reaction conditions to create a large array of compounds, allowing researchers to explore a vast chemical space efficiently. The resulting libraries facilitate the identification of novel compounds with desired properties, contributing significantly to the discovery and optimization of bioactive molecules and materials.

Presented by: Sihao Li *(Graduate, Biochemistry)*

Design and Synthesis of Sulfonyl-γ-AApeptide Building Blocks

γ-AApeptides are a new class of peptidomimetics that are currently being studied for potential applications in chemistry, biology, and medicine. They were first introduced in 2016 and have since been distinguished into different types of γ-AApeptides. From this we can reason that a process is in order to detail what are the necessary steps in the synthesis of these γ-AApeptides, specifically sulfonyl-γ-AApeptides. Sulfonyl-γ-AApeptides as a category of γ-AApeptides, is also distinguished by different building blocks. In which, designing a basic synthesis process procedure for sulfonyl-γ-AApeptide building blocks is imperative to serve as a guide for future reference and study.

Presented by: Sofia Mekouar *(Undergraduate, Biochemistry)*

Structure Study of Proline Cage

Proline cage is a project from Bo Huang and Sihao Li in our group. Proline cage can bind to halides and fluoride shows the strongest binding. My contribution is the crystallization part

and the XRD data is collected and analyzed by Dr. Wojtas. By crystallization, we found that self-cyclization happened in the final compound, and it led to an unwanted structure. After solving the self-cyclization problem, we got a disordered structure which is different from our design. Later, we obtained cocrystal with iodide.

Presented by: Cong Pan *(Graduate, Biochemistry)*

Emerging Nanoparticles-Mediated Gene Therapies Targeting Ocular Angiogenesis

This study explores non-viral nanoparticle-mediated gene therapy for controlling abnormal ocular angiogenesis in conditions like Diabetic retinopathy, and wet age-related macular degeneration. Conventional treatments face challenges, prompting the exploration of nanotechnology. Recent advancements in inorganic metal nanoparticles showcase effective angiogenesis control. Gene therapy offers a potential solution, though safety and efficacy issues persist. The review, focusing on wet age-related macular degeneration, highlights developments in pre-clinical and clinical studies. Proposed improved nanoparticle designs aim to enhance gene delivery efficacy, offering promising solutions for modulating angiogenesis and addressing vision loss challenges. Overall, nanoparticle-mediated gene treatments show significant potential in treating ocular angiogenesis.

Presented by: Pratyusha Samal *(Undergraduate, Biochemistry)*

Comparing Maestro/AutoDock Docking Scores with Experimental Data

This project was motivated by a lack of data necessary to correlate computational outputs with experimental expectations when designing novel photosensitive inhibitors. The goal of this project is to compare computational chemistry to experimental results. Specifically, we will analyze trends between the AutoDock and Maestro docking scores of popular protein ligand complexes and compare those values to experimentally determined docking values, such as the IC50 value for inhibitor drugs. Trend analysis will take into consideration the presence of certain amino acids, structure of the binding site, and structure of the ligand. If successful, this project will create a catalog for computational accuracy allowing for drug designers to better predict experimental results while designing new molecules.

Presented by: Aayush Singh *(Undergraduate, Biochemistry)*

Investigating the antimicrobial activity of sulfono-γ-AA peptides

The World Health Organization has designated antimicrobial resistance (AMR) as one of the top ten global health threats. Antimicrobial resistance occurs when bacteria, viruses and fungi evolve to no longer respond to available treatments. To combat this issue, novel treatments are needed. Biologically active peptides have been shown to have high receptor selectivity and binding potential as well as low toxicity. Using the chiral PNA backbone with side chain alterations at the γ carbon, we are able to show antimicrobial activity against MRSA.

Presented by: AnneMarie VanderSchouw *(Graduate, Biochemistry)*

Investigating the Effect of General Chemistry Pedagogy on Dimensions of Student Engagement Using AcES

Educational studies have shown that students learn better in active learning environments in comparison to traditional learning environments. With that information, this project aims to measure the differences in all dimensions of student engagement between peer-led and didactic lectures such as social, behavioral/cognitive, and emotional engagement. The effect of the pedagogy on a student's engagement while engaging in clicker questions during lecture periods will be determined using the Activity Engagement Survey (AcES). This can inspire future general chemistry courses to provide the most effective method of teaching, resulting in students with better overall performance in class. As an ongoing study, conclusions drawn from the final analysis of data can inform researchers and college instructors of the factors that contribute to a student's engagement in general chemistry courses. The findings of this study can support further educational developments in active learning.

Presented by: Bridget Dougherty *(Undergraduate, Chemistry Education)*

How the transition to remote learning in higher education was reflected in the learning centeredness of Physical Chemistry syllabi

Physical chemistry is perceived as a difficult course often because students find the content overwhelming, which leads to many misconceptions associated with the course, even after the students completed the class. The syllabus is often the first interaction students have with a course and its content can set the tone for their learning experience. A previous analysis of the learning-centeredness of physical chemistry syllabi revealed that the document is largely content-focused. The transition to remote instruction in response to the COVID-19 pandemic, led to significant changes in instructional strategies, as well as syllabi structure. This change led to our research which consisted of analyzing the extent of change in the learning-centeredness in physical chemistry syllabi using specific key identifiers in the rubric used for the initial analysis.

Presented by: Yara Khallaf *(Undergraduate, Chemistry Education)*

Examining ligand exchange rates in cobalt metal complexes via methods of conductivity and spectroscopic analysis.

Cobalt metal complexes have the ability to undergo a slow ligand exchange rate. Being able to isolate these products allows for the use of spectroscopic methods to analyze their compound properties. This study investigates the synthesis of various cobalt metal complexes and how their properties and ligand structures differ. A set of two cobalt coordination compounds was created via a multistep synthesis reaction involving the addition of several ligand-donating reagents. Methods of conductivity were used to show the direct relationship between conductance and ion concentration. Furthermore, infrared and UV-vis absorption spectroscopy allowed for ligand identification. The resulting data were used to draw conclusions regarding their electronic properties, charge, and ligand size.

Presented by: Nicholas Giunto *(Undergraduate, Inorganic Chemistry)*

Synthesis of Novel Hybrid Organic-Inorganic Halide Perovskite Materials

Halide perovskite semiconductors are one of the most versatile inorganic materials with applications in numerous fields. This research is aimed to synthesize these perovskites, and then to explore their applications to solar cells. For this applicability, synthesized materials must be semiconducting with low bandgaps. Novel syntheses were performed with various heavy metals paired with bulky organic linkers to modify the structure and increase stability. In this work, successful novel synthesis was achieved and the structure reported. Crystals were synthesized via a scalable hydrothermal synthesis method using organic linkers as well as through Teflon reaction vessel synthesis. The synthesized crystals were then characterized using primarily techniques such as X-ray Diffraction, Single Crystal X-ray Diffraction, but also Raman, photoluminescence spectroscopy, and thermogravimetric analysis. The synthesized materials were then tested for their stability in various environments.

Presented by: Brianna Pecourt *(Undergraduate, Inorganic Chemistry)*

Synthesis and Characterization of Novel Hybrid Metal Halides

The importance of semiconductor materials has been extremely prominent, particularly due to current material deficiencies for advanced applications. Metal Halides can be host to a unique variety of properties that, if explored, could revolutionize global issues such as energy, data storage, and climate change. One category of metal halides is that of hybrid halide perovskites. Hy-brid Perovskites can boast the usage of organic linkers that contribute to its wide spectrum of properties and limitless potential. In this work, we utilized a porous bulky organic linker [3.3.3 Cryptand] for metal halide synthesis using both direct precipitation and solvothermal methods. The employment of the porous organic linker is to supplement the water stability of the hybrid perovskite materials to improve environmental stability. In this work, we present the successful synthesis and structure for one of these materials.

Presented by: Brandon Sauval *(Undergraduate, Inorganic Chemistry)*

Hybrid Inorganic-Organic Metal Halides as Emerging Antimicrobial Agents

Metal compounds have been used for their medicinal properties for thousands of years and have excellent potential for combating antimicrobial resistance as a result of biological interactions that are difficult to replicate with purely organic molecules. Recent developments have indicated promise for hybrid inorganic-organic metal halides as antibacterial agents by controlling the production of ROS to inhibit drug-resistant bacteria. We have synthesized novel bismuth halide materials that exhibit intrinsic water stability as a result of their hydrophobic phosphine ligands, alongside inhibitory activity against both gram-positive and gram-negative bacteria. Further, these compounds exhibit excellent optical properties, with broad, band edge emission and have been determined to be excellent generators of Type I Reactive Oxygen Species (ROS), both in vitro and in vivo. These properties suggest a high potential for these materials to be used as antimicrobial agents.

Presented by: Sarah Troutt *(Undergraduate, Inorganic Chemistry)*

Stereospecificity of Tetracycline-Copper and Bacitracin-Copper Complexes on Oxidizing Catechin and Epicatechin

In this study, Tetracycline-Copper and Bacitracin-Copper complexes are employed as catalysts to investigate the stereospecificity of the complexes. Tetracycline is an oral antibiotic that treats an array of infections while bacitracin is a polypeptide antibiotic that is primarily used topically. The substrates in this study are two diastereomers, namely catechin and epicatechin, whose structures differ in only one chiral center. The reagents and the metal complexes were mixed in HEPES buffer, and the presence of 3-methyl-2-benzothiazolinone hydrazone (MBTH) helps trap the semiquinone generated by the oxidation reaction catalyzed by the aforementioned metal complexes. The formation of the quinones and their MBTH adducts(MBTH traps orthoquinone) are monitored by UV-vis spectroscopy. Both tetracycline-copper and bacitracin-copper complexes can distinguish catechin from epicatechin to certain degrees. And this study could help predict the fate of antibiotics in the environment.

Presented by: Guang Yang *(Graduate, Inorganic Chemistry)*

Isolation of Bioactive Secondary Metabolites from Mangrove Fungal Endophyte

Secondary metabolites are a subclass of natural products that make up a large portion of modern approved drugs. Endophytic fungi are a valuable source of secondary metabolites due to their interactions with their host and propensity to create anti-pathogenic compounds. Of these secondary metabolites, many exhibit antifungal properties against Candida albicans and Candida auris, two species of multidrug-resistant fungal pathogens that cause nosocomial infections resulting in high healthcare costs and mortality. The application of bioactive secondary metabolites from endophytic fungi provides a new source of antifungal drugs to combat the evolution of drug resistance and reduce the impact of infections. This project explores a fraction of an endophytic fungi sample (TAP14-275-DNMT-G), which was purified in a bioassay-guided manner. Purified secondary metabolites were then dereplicated and characterized, using LC-MS/MS and NMR data to identify known compounds through molecular networking.

Presented by: Emma Burdick *(Undergraduate, Organic Chemistry)*

Discussing the Synthesis and Utility of Amino Alcohols as Chiral Templates for Building Blocks in Peptidomimetic Cancer Research

Reducing amino acids to form promising amino alcohols for further alteration as applicable to more complex peptidomimetic reactions is the foundation of further pharmacological and biochemical synthesis. The formation and manipulation of these chiral alcohols are essential for future efforts. The focus of this study thus far has been to mass produce the amino acids of interest, reduce the present carbonyl to an alcohol, and use a dibenzylation process to benzylate the chiral product which is isolated for the subsequent bromination. This includes continued testing with dipeptides made of manipulated leucine and isoleucine; furthermore, alanine and glycine compounds are to be synthesized. This research is being conducted to develop novel artificial biomolecules to be utilized in applications of such important chiral derivatives. Further

alterations of these formed molecules include the use of these similarly structured non-peptide molecules as inhibitors of oncoproteins.

Presented by: Emma Cartwright *(Undergraduate, Organic Chemistry)*

Hydrogen Bonding Mediated Selective Recognition of Purine Bases by A Pyrrole Based [2+2] Molecular Cage in Aqueous Media

Molecular recognition of saccharides and heteroaromatics have been studied extensively where electrostatic interactions play a role in binding, especially for the charged substrates. Here we report synthesis of a [2+2] molecular cage containing four amide functionalities with two pyrrole units on the two ends and two tetramethyl substituted benzene rings on the sides facing parallel to each other. Due to the small binding cavity, the molecular cage does not capture carbohydrates, but the biomolecules containing five and six membered rings seem to fit well in the cavity due to their planar configuration and hydrogen bond donor atoms. Even though this macrocycle has its limitation in recognizing glucose, this is a stepping stone in designing simple molecular containers to recognize biogenic molecules such as hypoxanthine.

Presented by: Tobias Colmegna *(Undergraduate, Organic Chemistry)*

Discovery of purine-based CDK11 inhibitors for the treatment of breast cancer

CDK11 is known to play a critical role in the proliferation of different cancer cell lines, including breast cancer. Pre-clinical target validation studies demonstrate that genetic knockdown of CDK11 inhibits breast cancer cell growth, induces apoptosis, impairs tumor cell migration and invasion, and markedly inhibits tumor growth in vivo. We have developed a novel series of purine-based CDK11 inhibitors using structure-based drug design. The binding affinity in the series was confirmed using differential scanning fluorimetry, revealing preferred binding of S-enantiomer. This observation implies a stereochemical preference for the binding showcasing potential kinome-wide selectivity in the series. Furthermore, the inhibition was confirmed via radiometric kinase assay. These efforts are directed towards the discovery of potent, selective probes targeting CDK11, with the goal of elucidating the functions of these understudied proteins in pertinent breast cancer models in vivo.

Presented by: Nada Elkholy *(Graduate, Organic Chemistry)*

Isolation and Characterization of Novel Compounds from Endophytic Fungi

The increasing prevalence of antimicrobial resistance has led to an urgent need for the exploration of novel antimicrobial agents. Endophytic fungi have emerged in the world of natural products as a promising source for the discovery of bioactive compounds with potential antimicrobial properties. This study focuses on isolating and characterizing novel antimicrobial compounds from endophytic fungi. The research employs a multifaceted approach involving bioassay-guided fractionation and purification of active extracts, ultimately yielding individual bioactive compounds. Advanced analytical techniques, including nuclear magnetic resonance

(NMR) spectroscopy and mass spectrometry, are employed for the structural elucidation of isolated compounds. Subsequent evaluations encompass antimicrobial efficacy against different strains of Candida albicans and Candida auris.

Presented by: Zoe Flagg *(Undergraduate, Organic Chemistry)*

Efforts towards developing a synthesis of a computationally derived novel inhibitor of aminolevulinic acid synthase

Porphyria is a group of disorders that results from the body's inability to change porphyrins into heme. Currently, there are no medical treatments that address the root cause of porphyria, only those who aid with symptoms. In the heme biosynthesis, aminolevulinic acid synthase (ALAS) is the enzyme that catalyzes the first step. Previous studies have suggested that targeting ALAS could lead to the development of novel treatments of porphyria. HITS AI, a deep learning model, was used to generate compounds structurally different from previously explored. These compounds were created based on binding free energy and the predicted ability to inhibit ALAS. To test the accuracy of HITS AI, a compound was selected from a library of compounds developed by other labs at USF, such as Gloria Ferreira's lab. This process contributed to the efforts of making the desired compound and the synthesis is still being explored.

Presented by: Haley Gartrell *(Undergraduate, Organic Chemistry)*

Mild and Efficient Cs2CO3-Promoted Synthesis of Silyl Carbonates and Silyl Carbamates

Silyl carbamates and carbonates are ubiquitous compounds that hold a wide array of uses as pesticides, serve as novel protecting groups, and possess interesting medicinal applications such as peptidomimetics. Their biological applications include an introduction into partial structures of drugs to improve their efficiencies. A novel phosgene-free method and environmentally benign synthesis of silyl carbonates and silyl carbamates were developed via a three-component coupling of an amine or alcohol, carbon dioxide, and a trialkyl or trialkylsilyl halide. Cesium carbonate promoted not only successful carbonylations of alcohols and carbamations of amines but also suppressed common side reactions traditionally seen using existing protocols. Various alcohols and amines were examined, using a wide array of trialkyl-, triaryl halides, or sulfonates, respectively. In the future, a solid phase synthesis of the title compounds will also be investigated.

Presented by: Phillip Gray *(Undergraduate, Organic Chemistry)*

Optimization of a Hexenoic Acid Synthesis for Cannabinoid Analog Production

Currently, cannabinoid compounds, such as tetrahydrocannabinol (THC) and cannabidiol (CBD) exhibit minimal analog development. However, our group was able to develop a refined synthesis to optimize a rapid large-scale production of novel THC and CBD analogs. The synthesis can be obtained by synthesizing a hexenoic acid derivative as an intermediate. Since this intermediate

is the limiting step to the synthesis, developing a rapid and scalable synthesis is crucial. With our approach, we were able to make the transition from a four-step to a one-step synthesis of hexenoic acid enabling the exploration of a diverse library of novel cannabinoids. These synthesized analogs can then be tested against the cannabinoid receptors one and two as well as GPCRs for biological activity.

Presented by: Amanda Cimmini Hirata *(Undergraduate, Organic Chemistry)*

Synthesis of a family of optically pure benzyl and aliphatic α-hydroxyglycines

Peptidyl-Alpha-Hydroxyglycine Alpha-Amidating Lyase (PAL) conducts the conversion of α-hydroxyglycines into glycine amides and glyoxylates. These glycine amides are then used in the synthesis of peptide hormones and fatty acid amides. However, the enzyme only recognizes and processes only α-hydroxyglycines thus little of PAL substrates range and catalytic characterization have been investigated due to lack of pure testable substrates. Here a theoretical synthetic route for preparing optically pure PAL substrates is proposed, along with current experimental progress in the synthesis of benzyl and aliphatic α-hydroxyglycine substrates.

Presented by: Ethan Holitzner *(Undergraduate, Organic Chemistry)*

Isolating and identifying novel secondary metabolites for medicinal purposes

C. albicans and C. auris are nosocomial yeast infections with a high mortality rate and antimitotic resistance. Candida is responsible for two different diseases known as candidemia and candidiasis. Candidemia develops in immunocompromised patients upon exposure to infected objects or surfaces and has a mortality rate range of 30-60%. This has led to a demand for effective treatment for this disease and many studies for the treatment of antimitotic resistant infections. Endophytic fungi have millions of years of experience producing secondary metabolites that are designed to defend themselves from other fungi and inhibit the growth of competitors. Harnessing this design, secondary metabolites can be used as a source of new antimitotics. Using a high throughput screening method, bioassay guided fractionation of a fungal extract from a strain of Lasiodiplodia was done to find novel compounds with antifungal characteristics.

Presented by: Jackson Killian *(Undergraduate, Organic Chemistry)*

Development of 7-azaindole ULK1/2 kinase inhibitors as a potential therapeutic strategy to curb KRASG12C-driven NSCLC.

Lung cancer, the abnormal proliferation of lung cells leading to metastasis, ranks as the second most common cancer and primary cause of death in the US. Non-small cell lung cancer (NSCLC), comprising the majority of cases, often harbors KRAS mutations, notably KRASG12C. While FDA-approved inhibitors like sotorasib target this mutation, resistance mechanisms, limit their efficacy. Genetic mouse models demonstrate that autophagy is strikingly important in the survival and growth of RAS-driven cancers. Our lab's investigation into autophagy inhibition

led to the discovery of MR-2088, a potent and selective reversible ATP competitive inhibitor of ULK1/2, demonstrating excellent cellular target engagement and autophagy flux inhibition. Here we show our efforts to optimize bioavailability and overall pharmacokinetic (PK) properties in the series, aiming to enhance the therapeutic exposure of in-house ULK1 inhibitors.

Presented by: Micheal Lamptey *(Graduate, Organic Chemistry)*

Exploration of Bioactive Compounds from Hyalodendron Genus

This research investigates the Hyalodendron genus and bioactive compounds produced by it; utilizing a methodology, extraction, and MPLC/HPLC purification in a bioassay guided study. These samples are meticulously partitioned to eliminate any primary metabolites and therefore leads to an enhanced specificity in the latter analyses. The fungal sample is grown under three different epigenetic modifiers (DNA Methyltransferase, Nicotinamide, Butyrate) and a control sample. The isolation of bioactive compounds is achieved through MPLC and HPLC purification and the bioassay is important to test the compounds in potential therapeutic applications. The therapeutic application is replicating the resistance the samples have on Candida, which is a fungal species. The bioactive compounds will then be subjected to Spectrometric and spectroscopic analyses such as High Resolution Mass Spectrometry and Nuclear Magnetic Resonance with 1D and 2D experiments.

Presented by: Balaji Lingamgunta *(Undergraduate, Organic Chemistry)*

Synthesis of Activity-Based Probes of Palmitoyl Amides

Fatty acid amides (FAA's) serve as a type of endogenous signaling compound with diverse physiological functions. Notably, anandamide is an endocannabinoid with analgesic and anti-inflammatory properties, while oleamide contributes to sleep regulation. Despite their significance, the complete range of FAA functions and biosyntheses remains elusive. Through innovative probe design and advanced proteomic techniques, key proteins and interactions can be uncovered providing insights into the modulation of FAA signaling.

Presented by: Sian Marin *(Graduate, Organic Chemistry)*

Synthesis of a Biogenic Aldehyde, 3,4 Dihydroxyphenyl-acetaldehyde (DOPAL), a ToxicDopamine Metabolite in vivo: Implications for Parkinson's Disease Pathogenesis

Parkinson's Disease (PD) is one of the most common neurodegenerative disorders that affects roughly 2% of individuals over the age of 65. Pathologically the disease occurs by the loss of dopaminergic nerve cells located in the substantia nigra. These cells are responsible for the production of dopamine. With the loss of the brain region an individual is succumbed to the classical signs of PD, that being bradykinesia, tremors, and postural rigidity. The true cause of PD is still relatively unknown; however, a hypothesis is believed that catechol metabolites play a large role in dopaminergic nerve loss. DOPAL has been directly linked to neurotoxicity

and the PD disease state. The present research includes the use of the protecting group (THP) followed by the Witting reaction. The THP protecting group is used in order to provide stability to the molecule so reduction to the aldehyde may be pursued. The overall yield is expected to be higher than our past results.

Presented by: Savannah Page *(Undergraduate, Organic Chemistry)*

Facile multigram synthesis of preclinical CDK12-cycK inhibitor and molecular glue degrader SR-4835

SR-4835, a purine-based CDK12/13 inhibitor and molecular glue degrader, is currently under preclinical investigation for triple negative breast cancer treatment and is sold commercially for use in biological research. While its existing synthetic route serves medicinal chemistry-scale needs, enhanced in vivo efficacy and preclinical pharmacokinetic studies necessitate a more efficient multigram-scale route. The current method suffers from low atom economy and reliance on flash column chromatography for intermediate purification, limiting its suitability for large-scale production. Herein, we report a decagram synthesis of SR-4835 designed for enhanced scalability and operational simplicity. This optimized route utilizes readily available and cost-effective starting materials and reagents, achieving superior atom economy through six-step reaction sequences. This efficient and scalable synthesis significantly facilitates the production of SR-4835 for future in vivo applications.

Presented by: Manuel Manzanares Rodas *(Undergraduate, Organic Chemistry)*

Anion Recognition in Water using a Tetralactam Macrocycle

Throughout the years, there has been an increase in antibiotic resistance in cells. Through the study of anion recognition in water, many medical advances can occur, such as recognizing glucose in the body to help research in Type 2 Diabetes, or recognizing anions within cells. The goal is to design a macrocycle [host] that can function in an aqueous environment to bind through amide bonds with a selective guest. The binding is tested by NMR Titration, ITC, UV-Vis and through pH testing.

Presented by: Luzelena Sagal *(Undergraduate, Organic Chemistry)*

Synthesis of Bioactive Sulfonimidamides in Enantiopure form using Chiral SuFEx reagent t-BuSF

Sulfur (VI) functional groups have been a focal point in cancer research because they have many chemical benefits. Specifically, the enantiopure chiral S(VI) functional groups. These synthesized compounds are being used in clinical trials, with this comes a few tactical issues that need to be settled. One challenge is that the Sulfur (VI) functional groups have issues with controlling their stereochemical properties. This is where the Lopchuk research team is focusing its efforts on the development of a bench-stable, trifunctional, enantiopure, chiral S(VI) compound. Starting with the t-BuSF reagent, where it is possible to manipulate two different sulfur sites on a compound,

it must be scaled up. Using the prepared reagent many sulfoximines will be made from different aryl-lithium. These sulfoximines are then transformed into sulfonimidamides. These compounds have amine groups. Once the desired product is reached it is verified by the analytical methods of HNMR, 13C NMR, etc.

Presented by: Anna Sepulveres *(Undergraduate, Organic Chemistry)*

The Modified Piancatelli Reaction - A New Carbon-Carbon Bond Forming Reaction

Developing innovative and novel methods for carbon-carbon bond formation make up the backbone of organic chemistry and furthers advancement within the scientific and industrial fields. The Piancatelli rearrangement is a novel reaction that generates cyclopentenones from furfuryl alcohols through a furan ring opening-4π electrocyclization process. This reaction, however, is limited as it requires alcohol to be the nucleophile to form the ether. The use of a carbon-based nucleophile is being explored to generate a similar product, but the acidic conditions that accompanies the Piancatelli reaction presents a challenge as it is not a commonly seen occurrence for carbon-based nucleophiles. It is believed that enols could be a solution to this problem; therefore, this novel carbon-carbon formation is currently being pursued.

Presented by: Savannah Sharma *(Undergraduate, Organic Chemistry)*

Application of Unnatural Amino Acids to Understand Effects on Protein Structure and Folding Mechanisms

The many roles of proteins are made possible by the diverse interactions of their amino acids and the environment they exist in. The introduction of unnatural amino acids (UAAs) to protein structures by site-selective methods allows for changes in protein structure and function, opening the door for greater understanding of these complicated macromolecules and the tasks they can perform. Site selective methods also help make photoswitchable amino acids feasible allowing for light-induced isomerization of UAA introduced azobenzene derived side chains. In conjunction with analytical techniques including UV-vis and CD spectrometry, UAAs help to characterize conformational changes of proteins and the mechanisms by which these processes occur.

Presented by: Austin Barkley *(Undergraduate, Physical Chemistry)*

Exploring the Photoswitchable Properties of Azobenzene-BAPTA molecule and its Interaction with Calcium in Biological System

Biological events are the result of spatially and temporarily regulated cellular processes. Ca^{2+} ions concentration is essential for many of these processes. Calcium plays a fundamental role in muscle contraction, as a secondary messenger, neurotransmitter, nonmuscle motility, etc. BAPTA is a chelating agent to Ca^{2+} ions. However, Ca^{2+} binding to BAPTA is not reversible, and thus does not allow active modulation of the Ca^{2+} construction. Therefore, we have designed a BAPTA-like molecule that incorporates an azobenzene motif to create a photo switchable chelating agent for Ca^{2+} ions. Light-induced isomerization of the azobenzene will alter the

structure of the chelator, affecting its affinity to Ca^{2+} ions. The introduction of azobenzene will allow remote, instantaneous, and highly precise modulation of calcium concentration. The newly designed photoswitchable chelator will allow light-triggered regulation of cellular processes, and their dynamics with high time resolutions.

Presented by: Hafiza Zahra Rab Nawaz *(Graduate, Physical Chemistry)*

Identifying Binding Hot Spots on Protein Surfaces by Mixed-Solved MD and Flood Map Analysis.

Structure-based drug design (SBDD) process relies upon the identification of binding sites within therapeutic targets that possess the ability to modulate biological functionality. Mixed-solvent molecular dynamics (MixMD) simulations method utilizes small organic molecules to probe for potential binding pockets at the atomic scale and have recently undergone a surge of development among practitioners aiming to reinforce computational drug discovery efforts. The utility of MixMD simulations lies in the mapping of "hot-spots" within the biological targets where the probe molecules display high-affinity. In this research work we describe the development of flood map, a density-convolution algorithm that enables the computation of grid-free energies from MixMD simulations to guide downstream SBDD techniques. Here, we report the results of flood map in the context of the therapeutic target and study the potential presence of cryptic pockets in proteins, thrombin and beta-lactamase.

Presented by: Rajesh Paudel *(Graduate, Physical Chemistry)*

Restarting CHARMMing: Revising the CHARMM Web App

Updates to the computational chemistry web app, CHARMMing, are discussed. CHARMMing is a web app that simplifies the usage of CHARMM, a macromolecule modeling package. Development on CHARMMing stopped in 2017, and left behind two versions. "Old CHARMMing" is stable, but has relatively limited performance and functionality. In comparison, "New CHARMMing" is unfinished, but would have improved performance and functionality. The primary goals of this project are to host an instance of Old CHARMMing, and ensure it can be used for a variety of purposes without needing to excessively customize it. Secondary goals include deciding which version of CHARMMing should be used going forward, ensuring the future development and usage of CHARMMing is easier, and replacing any end-of-life software with modern, actively supported software.

Presented by: Michael Powell *(Undergraduate, Physical Chemistry)*

Structural analyses of uracil containing dsDNA sequences with XCUY motifs

Uracil is a common DNA lesion which is caused by spontaneous deamination of cytosine or misincorporation during replication. Previous studies in our laboratory have shown that certain uracil-containing dsDNA sequences undergo a register shift, where, upon base flipping of uracil, its orphaned complementary base will base pair with the base vicinal to uracil. These register

shifted structures are thought to be important for DNA repair, since they sterically block uracil from reentering the helix stack. To quantify register shifting propensities, molecular dynamics simulations were performed on 32 dsDNA sequences with XCUY motifs. Our simulations show that register shifts occur more frequently when the 3' or 5' nucleotide vicinal to uracil is a cytosine, although register shifted structures with thymine appear to be more stable. Structural and dynamical properties of register shifted sequences are presented.

Presented by: Maria Roallos *(Undergraduate, Physical Chemistry)*

Register Shifts in Uracil-Damaged DNA

Uracil is a highly mutagenic and common lesion of DNA, which is caused by misincorporation or spontaneous deaminating of cytosine. Uracil will spontaneously base flip, breaking its Watson-Crick hydrogen bonds and base stacking and leaving the helix stack. We previously observed that in rare cases, base flipping of uracil can be accompanied by a register shift, which sterically blocks the uracil from flipping back into the helix. To quantify the propensity of register shifts, we performed molecular dynamic simulations of 48 DNA sequences with central uracil-containing motifs. In these simulations, uracil was artificially flipped extrahelically toward either the major or minor groove. We confirmed wide occurrence of register shifts and characterized structural effects. Our study shows that register shifts most commonly occur for 3' cytosines on the uracil strand. Implications for DNA repair are discussed.

Presented by: Megan Tran & Bruno Young de Castro *(Undergraduate, Physical Chemistry)*

Spectroscopic studies of Equine Heart Myoglobin Mineralized in a Zeolitic Imidazole Framework

In progress towards sustainability, materials and methods to improve industrial processes and drug delivery are being explored. A promising material for biocatalyst, biosensing and drug delivery applications are heme proteins immobilized within Metal Organic Frameworks (MOFs). Preliminary studies have shown MOFs to enable proteins to retain biological functions in conditions that would normally cause denaturing. However, little is known about the effects of mineralization on protein structure. In this project, equine heart myoglobin was mineralized within a zeolitic imidazole framework, ZIF-8. Myoglobin contains a single protoporphyrin heme that reversibly binds small ligands like O2, CO, and NO. UV-Vis spectroscopy, tryptophan emission and transient absorption spectroscopy were used to determine if myoglobin is encapsulated and if myoglobin can bind and release CO. These techniques also offer valuable insight into the conformation of myoglobin and its functionality once encapsulated.

Presented by: Mason Weaver *(Undergraduate, Physical Chemistry)*

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