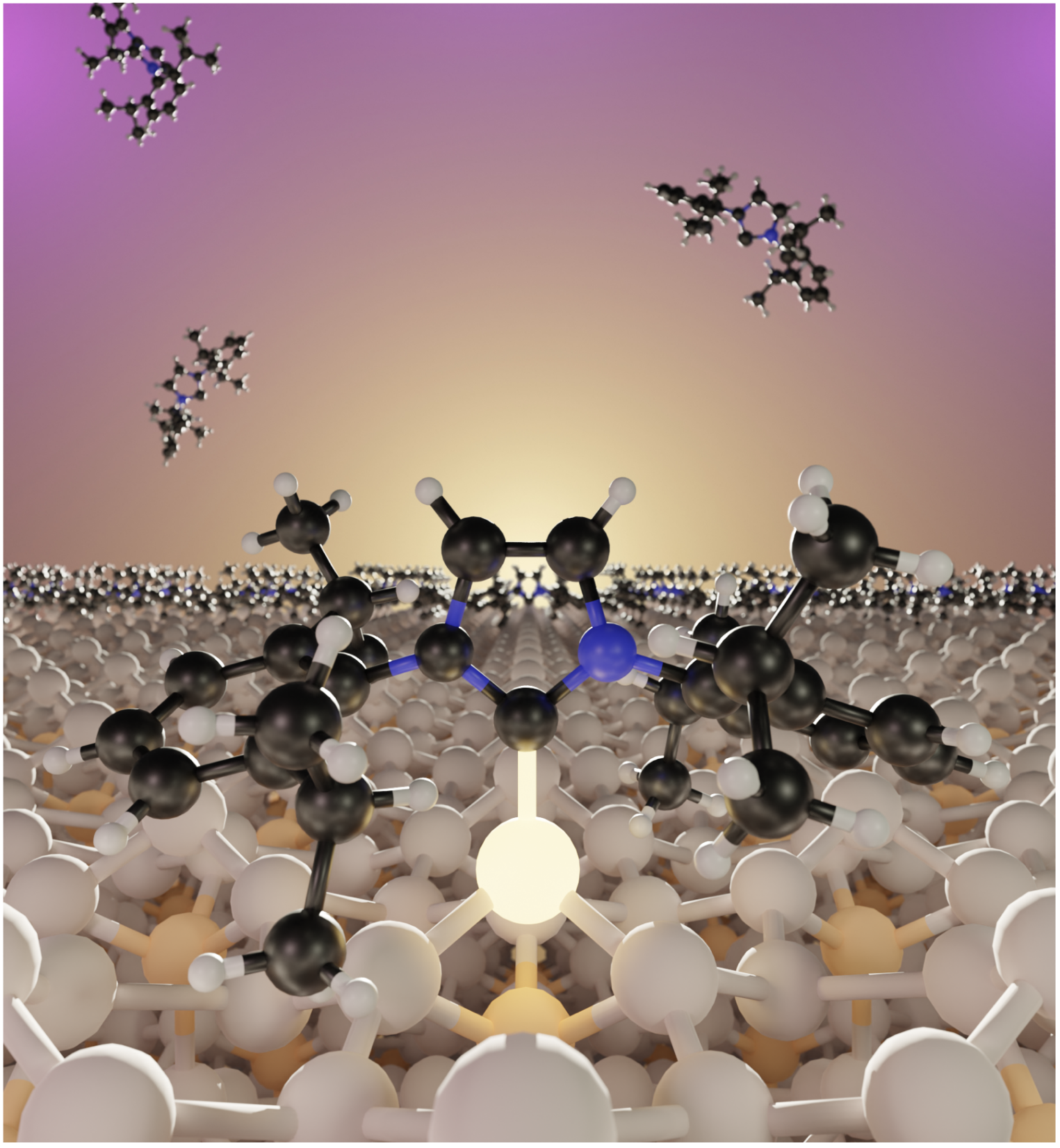
21st Annual
March 4, 2023

# Raymond N. Castle
## Student Research Conference



UNIVERSITY of SOUTH FLORIDA
Department of CHEMISTRY

castleconf.org

Cover art was inspired by the nature chemistry cover Vol. 13 No. 9. It showcases adsorption of N-Heterocyclic carbenes (NHCs) on silicon. Understanding how NHCs bind to silicon surfaces has paved the way for new electronic applications and is of upmost importance in the semiconductor industry. Nature Chemistry volume 13, pages 828–835 (2021)

Cover Art: Julian Melendez

Cover Design: Guy W. Dayhoff II

# 21st Raymond N. Castle Student Research Conference

**Saturday, March 4th, 2023**

Department of Chemistry, University of South Florida


# Table of Contents

# Agenda

---

**Breakfast and Registration** 08:00am - 09:00am
*(ISA 7th Floor)*

**Oral Session A** 09:05am - 11:15am
*(ISA 3048)*

**Oral Session B** 09:05am - 11:15am
*(ISA 3050)*

**Oral Session C** 09:05pm - 11:15pm
*(ISA 2023)*

**Lunch** 11:20am - 01:20pm
*(ISA 7th Floor, Jersey Mike's Subs)*

**Poster Session/Competition** 12:00pm - 01:20pm
*(ISA 7th Floor)*

**Oral Session D** 01:30pm - 03:20pm
*(ISA 1051)*

**Oral Session E** 01:30pm - 03:20pm
*(ISA 1061)*

**Castle Introduction** 03:30pm - 03:45pm
*(ISA 1061, Edward Turos, Ph.D.)*

**Plenary Presentation** 03:45pm - 04:45pm
*(ISA 1061, Marilyne Stains, Ph.D.)*

**Award Ceremony** 04:45pm - 05:00pm
*(ISA 1061)*

**Chemistry Bowl** 05:00pm - 06:00pm
*(ISA 1061 - 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, Marilyne Stains Ph.D.

As a discipline-based education researcher (DBER), Marilyne Stains focuses on characterizing the extent, nature, and factors involved in the gap between instructional practices in science college classrooms and education research. Stains is specifically interested in exploring how instructors think about their teaching, as well as identifying individual, departmental, and institutional factors that influence instructors' teaching decisions.

Stains' work has been published in Science, CBE-Life Sciences Education, and the Journal of Chemical Education. She has received funding from the National Science Foundation, including a CAREER award (2016). In 2019, she was awarded the Presidential Early Career Award for Scientists and Engineers (PECASE) and the American Chemical Society Women Chemists Committee Rising Star Award.

Stains received her B.S. in Chemistry from the Université des Sciences de Luminy, France; her M.S. in Chemistry from the Université Paul Sabatier, France; and her Ph.D. in Chemistry from the University of Arizona. She conducted her postdoctoral studies at the University of Massachusetts Boston. She started her academic career at the University of Nebraska-Lincoln in 2011 and was promoted to Associate professor with tenure in 2016. Stains joined the Department of Chemistry at the University of Virginia in August 2019 and was promoted to full professor in 2022.

## Plenary Presentation

**Exploring General Chemistry instructors' rationales behind their assessment practices**

Instructional innovations and reforms over the last decades have been mostly focused on practices to engage students with the materials in the classrooms. One aspect of instruction that plays a key role in learning but that has been overlooked in these reform efforts is assessment. Students use their instructor's assessment practices to identify what instructors values and therefore to prioritize their studying. Recognizing the influence that assessment plays in student learning, chemistry-based education researchers have been advocating for the implementation of new assessment approaches that can support the development of students' content knowledge and scientific practices. In order to help the propagation of these new approaches, we first need to understand chemistry instructors' thinking about assessment practices. In this study, we explored 19 general chemistry instructors' rationales for their assessment practices. These instructors come from 14 different institutions across the United States of America. We describe their assessment practices, their views on the purpose of assessment, and the alignment between this purpose and their practices. Finally, we also explore external influencers that affect their assessment practices.

# Oral Session Breakdowns

---

## Oral Session A (ISA 3048)

| | |
|---|---|
| Lei Wang | 09:05am - 09:25am |
| Ali Azmy | 09:25am - 09:45am |
| Jessica "J.D." Young | 09:45am - 10:05am |
| ***intermission*** | 10:05am - 10:15am |
| Benjamin Smith | 10:15am - 10:35am |
| Nadja Bijelic | 10:35am - 10:55am |
| Chengkai Xu | 10:55am - 11:15am |

## Oral Session B (ISA 3050)

| | |
|---|---|
| Isaiah Nelsen | 09:05am - 09:25am |
| Brianna Jones | 09:25am - 09:45am |
| Ernesto Arcia | 09:45am - 10:05am |
| ***intermission*** | 10:05am - 10:15am |
| Briley A. Humphrey | 10:15am - 10:35am |
| Robert Feeney | 10:35am - 10:55am |
| Sang Phan | 10:55am - 11:15am |

## Oral Session C (ISA 2023)

| | |
|---|---|
| Alissa Anderson | 09:05am - 09:25am |
| Dianna Kim | 09:25am - 09:45am |
| Jenny Williams | 09:45am - 10:05am |
| ***intermission*** | 10:05am - 10:15am |

| | |
|---|---|
| Meng Gu | 10:15am - 10:35am |
| Vishala Maharaj | 10:35am - 10:55am |
| Cameron Murray | 10:55am - 11:15am |

## Oral Session D (ISA 1051)

| | |
|---|---|
| Ayesha Farheen | 01:30pm - 01:50pm |
| Xue Zhao | 01:50pm - 02:10pm |
| Sarah G. Dietrick | 02:10pm - 02:30pm |
| ***intermission*** | 02:30pm - 02:40pm |
| Julian Melendez | 02:40pm - 03:00pm |
| Mohammad Nazmus Sakib | 03:00pm - 03:20pm |

## Oral Session E (ISA 1061)

| | |
|---|---|
| Nathaniel Schmidt | 01:30pm - 01:50pm |
| Christian Sabbagh | 01:50pm - 02:10pm |
| Katrinah Tirado | 02:10pm - 02:30pm |
| ***intermission*** | 02:30pm - 02:40pm |
| Paul Orndorff | 02:40pm - 03:00pm |
| Abrun Swanson Nereim | 03:00pm - 03:20pm |

# Oral Presentation Abstracts (Morning - Session A)

---

**Development of the safe and broad-spectrum aldehyde and ketoamide Mpro inhibitors derived from the constrained $\alpha$, $\gamma$-AApeptide scaffold**

In the last two decades, three highly pathogenic coronaviruses known as SARS-CoV, MERS-CoV and SARS-CoV-2 emerged. Among them, SARS-CoV-2 is still wreaking havoc all over the world with surging morbidity and high mortality, necessitating the urgent need to develop new antiviral drugs with broad-spectrum activity. The main protease (Mpro) is a viral cysteine protease involved in the cleavage of polyproteins pp1a and pp1ab, which is essential in the replication of SARS-CoV-2, enabling Mpro an active target for antiviral development. Herein, we reported the design and synthesis of a new class of peptidomimetics-constrained $\alpha$, $\gamma$-AApeptides, based on which a series of aldehyde and ketoamide inhibitors of the Mpro of SARS-CoV-2 were prepared. The promising compounds showed excellent inhibitory activity in the FRET-based Mpro enzymatic assay not only for the Mpro of SARS-CoV-2 but also for SARS-CoV and MERS-CoV, along with HCoVs like HCoV-OC43, HCoV-229E, HCoV-NL63 and HKU1.

*Presented by: Lei Wang* *(Graduate, Biochemistry)*

**Porous and Water Stable 2D Hybrid Metal Halide with Strong Broad Light Emission and Selective $D_2O$ Adsorption**

Halide perovskites are a unique class of semiconductor materials with intriguing optoelectronic properties; this family of materials have the potential to be suited for a wide array of applications such as photovoltaics, LEDs, and radiation detection.Developing water stable perovskites and metal halide materials has been a highly sought-after property as it will allow their utilization in unexplored for them applications such as solid-state batteries and photocatalysis. Towards this challenge, we report a strategy for generating porosity in hybrid metal halide materials by using molecular cages serving as both structure-directing agents and counter-cations. Reaction of the [2,2,2] cryptand (DHS) linker with Pb (II) gave rise to the first porous and water stable 2D metal halide semiconductor $(DHS)_2Pb_5Br_{14}$. The material is a direct bandgap semiconductor and is water stable for more than a year.

*Presented by: Ali Azmy* *(Graduate, Inorganic Chemistry)*

**A Four-DimensionalConceptualization of First-Year Chemistry Students' Sense of Belonging**

A person's sense of belonging is their connectedness, inclusion, and relationship with others and their general environment. As well, it is context-specific. Despite this, an investigation specific to how students perceive and achieve a sense of belonging in the chemistry class environment has not been conducted. Such explorations are necessary to understand how instructors can promote students' affect,motivation, and wellbeing. To address this gap in the literature, 19 postsecondary students from first-semester general chemistry or a preparatory chemistry course

were interviewed. To start the interview, students ranked 16 belonging statements. Then, a semi-structured interview was conducted to explore the students' reasoning behind their ranking. Qualitative analyses developed four belonging dimensions. This nuanced understanding will improve students' sense of belonging within chemistry courses through intentional instructional practices and further research on sense of belonging.

*Presented by: Jessica (J.D.) Young* *(Graduate, Chemistry Education)*

**New p-hydroxyphenylimidazole metabolites from the Florida Keys sponge Phorbas sp.**

With the application of GNPS, a molecular networking tool, four new p-hydroxyphenylimidazole metabolites were isolated and characterized from Phorbas sp. collected in the Florida Keys. Mass clusters in the molecular network are based on matching MSMS fragmentation patterns observed on the LCMS-QTOF. Nocapanazole A-D share the same p-hydroxyphenylimidazole structure as amaranzole steroids B, E and F; however, these new structures contain different alkyl chains instead of the steroid backbone. Bioinformatic platforms available online suggest nocapanzole a-d have strong inhibition against Mycobacteria tuberculosis. Bioactivity is currently being evaluated against Candida spp. No bioactivity was found against ESKAPE pathogens.

*Presented by: Benjamin Smith* *(Graduate, Organic Chemistry)*

**Syntheses of a Biochemically Important Aldehyde, 3,4-Dihydroxyphenyl- acetaldehyde (DOPAL), a Toxic Dopamine Metabolite in vivo: Implications for Parkinson's Disease Pathogenesis**

3,4-Dihydroxyacetaldehyde (DOPAL) when injected into rat brains results in neuronal cell death that is more selective for cells in the substantia nigra (cells which are primarily dopamine-producing cells). Despite the significance of DOPAL, it is scarcely commercially available and must be synthesized. There are several published methods, but they all share one common problem. DOPAL is very unstable and is very difficult to isolate and work with. In an early, reported synthesis, DOPAL was isolated in four steps, three chromatographic separations, and proceeded with an overall yield of about 4%.

*Presented by: Nadja Bijelic* *(Undergraduate, Organic Chemistry)*

**Ion-Diople Interaction: An Overlooked Tool to Design and Synthesize Acyclic Receptors for Lithium with High Binding Affinity and Selectivity**

Lithium has become increasingly in demand due to its wide range of applications. To address this issue, the development of molecular receptors that can effectively recognize, sense, extract and purify Lithium cation is essential. Previous development on Lithium receptors was based on the principle of pre-organization and size match, especially macrocyclic receptors. High affinity has been achieved, but Li+/Na+ binding selectivity is limited. Acyclic receptors was easier to synthesis, and was proved to have good sensing ability on ion selective electrode. However, the

affinity and selectivity of them remains unclear and unexplained. We conducted a systematic evaluation of acyclic lithium receptors and found electronegativity of the binding sites is an overlooked factor that affects binding affinity and selectivity of Li+.

*Presented by: Chengkai Xu* *(Graduate, Organic Chemistry)*

# Oral Presentation Abstracts **(Morning - Session B)**

---

**Patterns of Reasoning: Acid and Base Strength**

In organic chemistry, acids and bases represent a foundational topic essential to the understanding of many reactions taught thereafter. Assessing student knowledge on acid/base strength has been of particular interest within chemical education literature in an attempt to deepen understanding of student conceptions and approaches to this topic. In this study, student knowledge of acid/base strength is explored with emphasis on the patterns of reasoning utilized throughout various tasks. Throughout the tasks, students use both structural and electronic features as a method for discerning the most acidic/basic molecule when provided two structures. Students that centered their mental models around stability found greater success in providing support for their decisions. However, an overwhelming majority of students found difficulty in determining base strength, exposing a possible crack in the foundation of acid/base strength curriculum in organic chemistry.

*Presented by: Isaiah Nelsen* *(Graduate, Chemistry Education)*

**Characterization of Liposomes and Exosomes using Spectradyne**

Exosomes are extracellular vesicles ranging in size from 30-150nm. Loaded with biological molecules such as lipids, proteins, RNA and more, exosomes have become an emerging use for targeted drug delivery. A necessary step in this process is the characterization of exosomes. As not much is known about exosomes as a use for drug delivery, liposomes can be used as a reference standard. Both liposomes and exosome will be characterized using the Spectradyne, a nanoparticle analyzer. While characterizing these vesicles, the Spectradyne will also be used to validate Surface Acoustic Wave (SAW) technology for the disruption of lipid assemblies, which allows for analysis using mass spectrometry. 100nm DOPC liposomes, with and without Cholesterol will be lysed on the SAW at 0, 30, 60 and 90 seconds at a frequency of 64 mHz and compared.

*Presented by: Brianna Jones* *(Graduate, Analytical Chemistry)*

**Effect of E.coli gene deletions and antibiotic deactivating enzyme mutations on bacterial fitness**

Evolution of antibiotic resistance has become a big problem when trying to deal with bacteria that pose a threat to human health. In this project we examine the intermolecular epistatic effect between multiple E. Coli genes and a set of intermediates along the evolutionary pathway of antibiotic deactivating enzymes. A set of engineered E. coli cell lines were exposed to increasing antibiotic concentrations to determine the minimal inhibitory concentration (MIC), in order to use it as a fitness proxy. A total of 110 experiments were performed in duplicate, comprised of a combination of 22 strains and five evolutionary intermediates of the deactivating enzymes. The results show that the MIC of some of the strains have a statistically significant difference when compared to the wild type while others do not, suggesting that some genes have a bigger impact in facilitating evolution and survival compared to others.

*Presented by: Ernesto Arcia* *(Graduate, Biochemistry)*

**Development of novel JAK2 inhibitors and PROTACs for the investigation of JAK2 inhibition and degradation**

Janus kinase 2 (JAK2) is a protein kinase involved in the JAK/STAT pathway which is reported as one of the core cancer pathways; thus, the regulation of JAK2 is important in the maintenance of normal cell function. A fragment-based approach was taken to identify building blocks displaying potent biological activity and Schrodinger docking analysis was used to probe the binding interactions within the ATP binding site of JAK2. PROTACs were designed to investigate the degradation of JAK2 based on ligands that displayed high binding affinity. A pyrimidine and pyrrolopyrimidine core was exploited to explore hydrogen-bonding interactions within the hinge region of JAK2 to investigate binding affinity. A-ring and B-ring fragments were used to develop structure activity relationships with data obtained in functional assays and in-vivo cell viability assays. Several key inhibitors and PROTACs were identified to bind strongly to JAK2 and modulate JAK2 activity in appropriate cancer cell lines.

*Presented by: Briley A Humphrey* *(Graduate, Organic Chemistry)*

**Tools for Probing the Fatty Acid Amide Proteome**

Fatty acid amides make up a large, and diverse group of endogenous signaling compounds with an equally diverse range of functions. Members of the group like Anandamide, an endocannabinoid, and Oleamide, a sleep regulator, have been extensively studied. Even still, there is more to be learned about them and the hundreds of other fatty acid amides with functions and biosyntheses we do not fully understand. Affinity based proteomic probes have been synthesized in order to develop a broader understanding of the workings within the fatty acid amide system. This work focuses on the design and synthesis of these molecular tools.

*Presented by: Robert Feeney* *(Graduate, Organic Chemistry)*

**Investigation of Mad2 protein 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. Studies have shown Mad2 mutants only adopt one conformation. This blocked the crucial transformation required for the function of the spindle checkpoint. To gain insight into the effect of each mutant, we performed unrestrained MD simulations for 200 ns of normal and mutant variants of Mad2. By using a series of analysis such as RMSD, covariance, quasiharmonic modes, we aimed to find common patterns among the mutants. Additionally, we have calculated the conformation free energy difference between the two states of Mad2 using the focus confinement method. Biological implications will be discussed.

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

# Oral Presentation Abstracts **(Morning - Session C)**

---

**Hybrid Organic-Inorganic Perovskites: Towards Antimicrobial Resistance Applications**

Halide perovskites have a unique, defining structure with significant potential towards real world applications, such as solar cells and photocatalysis. Though traditional lead-based perovskites are typically toxic, by replacing the metal with a more biocompatible substitute, such as bismuth, copper, or antimony, we can produce biocompatible perovskites with similar optoelectronic properties. To do this, we implemented molecular and crystal engineering with existing organic antimicrobials for the development of novel perovskites using scalable synthesis methods to produce high quality single crystals, and modulate the structure to optimize their antimicrobial properties. Preliminary data indicates the successful formation of new crystal phases, while the determination of their structural and optoelectronic properties render them potential candidates for both antimicrobial agents and photodynamic therapies, beyond traditional applications for perovskites.

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

**Student Responses to Stoichiometry Problems and the Effect of Supplementary Tables as Potential Scaffolds**

Stoichiometry is an essential concept to student success in general chemistry, a prerequisite course for STEM fields. The inclusion of supplementary tables that model each chemical in a reaction contrasted with the differing measures of amount has shown improvements in student outcomes on this topic. This work investigated why the addition of a table results in improvements in student problem-solving. Open-ended stoichiometry survey prompts were delivered to

off-sequence first-semester general chemistry students and 415 responses were collected. The survey assigned students to randomly receive a table or no table for each prompt. Responses were analyzed by coding students' explicit use of labels, units, and procedures, and chi-square analyses were conducted to explore the impact of including tables. The inclusion of tables cued students to apply the mole ratio and chemical labels more, though the results were inconsistent across prompts.

*Presented by: Dianna Kim* *(Graduate, Chemistry Education)*

**Metabolomic Study of Archived Cnidarian Specimens from the Smithsonian National Museum of Natural History**

In this study, ethanolic extracts provided by the Smithsonian National Museum of Natural History (Washington, D.C.) were analyzed to create a metabolomic 'fingerprint' of various Cnidarian species – providing the means for the chemotyping of different phenotypes, forming chemotaxonomic assignments for undefined specimens, and proposing cryptic speciation. Using targeted nuclear magnetic resonance (NMR) and untargeted high resolution liquid chromatography tandem mass spectrometry (LC-MS/MS), metabolomic features were annotated by both manual inspection of spectra and AI-based programs. Statistical relationships among the samples and cheminformatics were assimilated via MetaboAnalyst, then applied towards chemotyping the selected samples.

*Presented by: Jennifer Williams* *(Graduate, Analytical Chemistry)*

**Peptidomimetic-based Amyloid beta 42 inhibitor mediating critical A$\beta$ inhibition and disassembling activity**

As the increasing proportion of elderly population, there could be around 78 million people with dementia in 2030 and 139 million in 2050 based on the WHO report. Plenty of therapeutic strategies have been explored to treat this kind of disease but to date, none of them showed satisfactory efficacy. It's still of prime importance to develop novel treatment strategies against AD. Herein, we report the A$\beta$ inhibitor H-C-9 demonstrating an excellent activity on not only inhibiting A$\beta$42 aggregation, but also disrupting A$\beta$42 aggregates already formed. In this study, various assays were conducted to investigate its ability of reducing toxicity of A$\beta$ aggregates

*Presented by: Meng Gu* *(Graduate, Organic Chemistry)*

**Acridinium Catalyzed Decarboxylative Amination of Diazirines**

Given the prevalence of nitrogen-containing compounds in medicine, agriculture, and materials, it is an ongoing challenge in synthetic organic chemistry to find efficient strategies for C–N bond formation. Our group is interested in synthesizing these compounds via a radical amination strategy using diazirines as an electrophilic nitrogen source. Previously, we reported two methods of performing decarboxylative aminations with diazirines and N-(acyloxy)phthalimides via transition metal catalysis or using mild photoactivators. These reactions were successful in providing substituted diaziridines that are used in making a wide range of heterocyclic compounds.

Building upon these results, decarboxylative photoredox reactions catalyzed by acridinium-based catalysts were tested. This reaction is expected to be useful for the late-stage modification of high value nitrogen-containing compounds without pre-functionalizing the starting carboxylic acids.

*Presented by: Vishala Maharaj* *(Graduate, Organic Chemistry)*

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

Porphyria is a class of disorders that is caused by the buildup of porphyrins in the body. So far, current medication only treats the symptoms of porphyria, not the root cause of the disease. Research suggests that by targeting aminolevulinic acid synthase (ALAS), the enzyme that catalyzes the first step in the biosynthesis of porphyrins, a viable drug to treat this class of disorders can be developed. Utilizing HITS AI, a deep learning model, a series of compounds were generated based on binding free energy that could inhibit ALAS. To verify this model a compound was selected for synthesis.

*Presented by: Cameron Murray* *(Graduate, Organic Chemistry)*

# Oral Presentation Abstracts **(Afternoon - Session D)**

---

**A variety of students' approaches while predicting the location of dipole-dipole intermolecular forces between two distinct molecules**

The different approaches students use in predicting intermolecular forces are presented to offer evidence of where students' misunderstandings with intermolecular forces might be stemming from. General chemistry students were given pairs of molecules and told that dipole-dipole forces exist between them. The task was to describe the atoms or parts of the molecules where the force exists and the reasoning behind their selection. Half of the students invoked an attraction of opposite charges, while some of those used electronegativity inappropriately to locate the charges. Other approaches include assigning the dipole-dipole forces to where there were atoms with an electronegativity difference, atoms with large electronegativity magnitudes, atoms with big atomic sizes, or within molecules that have a bent shape. The chemically inappropriate approaches could be used to create distractors in students' clicker questions to promote a more accurate understanding of intermolecular forces.

*Presented by: Ayesha Farheen* *(Graduate, Chemistry Education)*

**Design of stapled antimicrobial peptides that kill antibiotic-resistant bacteria**

The cationic alpha-helical antimicrobial peptides (AMPs) have been proposed as a potential solution to the global threat of multidrug resistance. However, AMPs have been clinically

hindered by structural instability, proteolytic degradation, in vivo toxicity, etc. Here we design and synthesize the stapled AMPs based on Magainin 2 using gamma-AA peptides' backbone that can selectively kill multidrug-resistant bacteria.

*Presented by: Xue Zhao* *(Graduate, Biochemistry)*

**Profiling drug-resistance of Candida spp.**

Drug-resistant pathogens, such as infectious fungi, are an increasing threat to humanity. To combat these deadly and evolving organisms, we explore a method for mapping drug susceptibility and resistance to various FDA approved drugs. A robust high-throughput growth inhibition screening allows for a "fingerprinting" profile of each drug across panels of two Candida species (C. auris and C. albicans). Marine organisms (including endophytic fungi, coral, tunicates, and sponges) were additionally screened to compare resistance profiles. Further analysis of scaled-up extracts and subsequent fractions was performed via nuclear magnetic resonance (NMR), liquid chromatography mass spectrometry (LC-MS). Dereplication was achieved through the use of online resources such as Global Natural Products Social Molecular Network (GNPS) and Small Molecule Accurate Recognition Technology (SMART).

*Presented by: Sarah G. Dietrick* *(Graduate, Organic Chemistry)*

**Improved Polarizable Force Field for Modeling Mg2+ Binding to Proteins and Nucleotides**

Magnesium is an indispensable regulatory cation for numerous cellular enzymes and membrane proteins that participate in a variety of biological processes, including cell signaling and genome stability. Molecular mechanics simulations have the potential to provide detailed insights into the mechanisms of these Mg-dependent proteins. However, MM force fields continue to suffer from large inaccuracies when dealing with divalent cations. The inclusion of explicit polarization in MM models, such as in CHARMM Drude and AMOEBA models, has been promising, but despite substantial improvements errors remain high. Toward addressing this long-standing challenge, we recently presented a recalibration of the AMOEBA model. Notably, polarization terms of cation-coordinating groups were improved to respond better to the high electric fields present near cations. This systematically reduced errors in interactions of monovalent cations with proteins. Here we show that this revised model, along with our many body NB-fix corrections, reduces errors in Mg2+-protein interaction energies to 6 kcal/mol from QM target data as well as improving interactions with ATP/ADP.

*Presented by: Julian Melendez* *(Graduate, Physical Chemistry)*

**Studies of Potential New Synthetic Ketogenic Molecules**

Ketosis is a metabolic state where liver produces small molecules called ketone bodies, that most cells in the body can use as a source of energy. Other than working as a source of energy during prolonged fasting or carbohydrate restriction ketosis has already an established treatment for

epilepsy and type 2 diabetes. Although, a good amount of research was done on ketogenic diet recent times, the field of synthesis of novel ketogenic compounds was neglected. Our endeavor was to find synthetic routes and characterization of some new small ketogenic molecules.

*Presented by: Mohammad Nazmus Sakib* *(Graduate, Organic Chemistry)*

# Oral Presentation Abstracts **(Afternoon - Session E)**

---

### Isolation and Structure Determination of Secondary Metabolites from Everglades Endophytic Fungi

Endophytic fungi occupy an ecological niche that makes them ideal organisms for the discovery of novel bioactive secondary metabolites. Fungi are well-known for their antimicrobial secondary metabolites, with these compounds having a profound impact on drug discovery over the past century. With the rise of multi-drug resistant pathogens, there is a compelling need for novel antimicrobial compounds to combat their proliferation. Our study aims to isolate and identify metabolites that are active against ESKAPE pathogens and drug resistant Candida albicans. Due to extensive study of fungal metabolites in the past, we employed the techniques of dereplication and chromatographic editing to rapidly identify and remove known metabolites at early stages of purification. This study has led to the isolation of several known and novel antimicrobial compounds. The structure elucidation of these secondary metabolites was achieved using a combination of 1D and 2D nuclear magnetic resonance (NMR).

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

### Carbinolamide synthesis project

This project seeks to synthesize novel carbinaolamides to use in enzyme kinetics experiments for the enzyme PAM (peptidylglycine alpha-amidating monooxygenase). This synthesis project seeks to determine first and foremost, whether the stereoisomer (R or S) will affect the rate of catalysis to the end product. The project also seeks to synthesize compounds that vary in hydrophilicity and other chemical effects to introduce new variables to the bifunctional enzyme reaction mechanism.

*Presented by: Christian Sabbagh* *(Undergraduate, Organic Chemistry)*

### Zinc mediated one-pot reductive acylation and silylation of various quinone derivatives

The reduction of p-quinones to hydroquinones is commonly utilized in nature for the design of biologically active molecules. Unstable hydroquinone variants can be challenging to isolate or even characterize under normal quinone reduction conditions as they are easily oxidized back to their quinone form or to other undesired by-products. Methods to reduce the quinone and

trap the hydroquinone products in one step may be an effective way to obtain the desired hydroquinone species in a form suitable for use as a prodrug. Our lab has examined a zinc mediated one-pot reductive silylation and acylation strategy to obtain photosensitive quinone derivatives in high yield using protecting groups. Characterization of these reduced protected hydroquinones will allow for further investigation into the development and design of new highly reduced prodrug molecules for use in pharmaceutical applications.

*Presented by: Katrinah Tirado* *(Graduate, Organic Chemistry)*

**Role of sequence on the flexibility of uracil damaged DNA**

Uracil is a common lesion in DNA which is recognized and removed by uracil DNA-glycosylase (UDG) as a part of the base excision repair pathway. UDG excises uracil by a base flipping mechanism, and the ease of this flipping motion depends on context of bases surrounding the site of damage. We hypothesize that UDG activity depends on the intrinsic deformability of the base steps neighboring the uracil. The rigidity of a diverse set of uracil-damaged and undamaged sequences have been studied and compared via molecular dynamics simulations. Measurements of bending persistence lengths, base step parameters and base flipping events have been studied and compared amongst different sequence contexts, and results display a correlation between global bending properties and flipping of the lesion site. To further study the link between DNA bending and base flipping, 2D umbrella simulations were executed on uracil containing sequences with results supporting trends in unbiased simulations.

*Presented by: Paul Orndorff* *(Graduate, Physical Chemistry)*

**Validation of the Multi-surface Adiabatic Reactive Molecular Dynamics Method**

The drug discovery process relies on efficient computational methods in order to identify promising compounds for further experimental evaluation. Molecular dynamics (MD) methods make it possible to efficiently screen large libraries of potential drug candidates but many fail to describe the breaking and formation of bonds along reactive pathways. One such MD-based method which is suitable for describing such systems with dynamic bond configuration is the Multi-surface Adiabatic Reactive Molecular Dynamics method (MS-ARMD). In this work, MS-ARMD is validated through the parameterization of the SN2 reaction between chloromethane and the chloride ion as well as the Claisen rearrangement of Allyl Vinyl Ether–both in gas phase. MS-ARMD was found capable of modeling the SN2 reaction of chloromethane. An ensemble of structures near the transition state of this SN2 reaction exhibits better overlap with energies calculated at a higher level of theory than is possible through traditional MD.

*Presented by: Abrun Swanson Nereim* *(Graduate, Physical Chemistry)*

# Poster Presentation Abstracts (Midday - Posters)

---

**Mass Spectrometric Analysis of Cytochrome C : Cardiolipin Complex**

Cytochrome c(cyt c) is a protein in the mitochondrial membrane. Its release contributes to triggering apoptosis. Cardiolipins(CL) play a key role in pro-apoptotic factors, such as the release of cyt c. The cyt c: CL complex results in conformational changes leading to a change in the mass-to-charge ratio of the complex.

*Presented by: Sarah Carroll - P29* *(Undergraduate, Analytical Chemistry)*

**Characterization of Liposomes using SEC-HPLC**

The goal of this project is to create a standard operating procedure (SOP) for the separation of liposomes using the Zenix SEC-100 (size exclusion column) on a high-pressure liquid chromatograph (HPLC). When making liposomes, the mixture includes the liposome, free lipid, and whatever is used to load the liposomes. In this study, loaded liposomes, unloaded liposomes, free lipid, and Cytochrome C (the drug used to load the liposome) is run on the HPLC to characterize the peaks seen in the chromatograph to show the separation of the components. Samples separated from the HPLC are collected and run-on dynamic light scattering (DLS) to verify the size of the liposomes separated by the HPLC.

*Presented by: Samantha Czerniakowski - P28* *(Undergraduate, Analytical Chemistry)*

**Optimization of the Solid-Phase Extraction Methodology of Human and Mice Urine via HPLC-QTOF Analysis.**

Across the life course, humans are exposed to external and internal factors that cause molecular modifications, such as DNA adducts, which may result in chronic diseases. The DNA adductome serves as a biomarker of the interaction between the exposome and the genome. To link human, environmental carcinogen exposure, and cancer risk with DNA modifications, adductome maps developed from HPLC-QTOF analysis serve as the non-invasive assessment of DNA adductomics via urine. The goals of this project are to: (1) Determine the concentration of DNA adducts of each column combination via HPLC-QTOF analysis, (2) Create DNA adductome maps of each column combination via HPLC-QTOF analysis, and (3) Determine the optimal column combination for the double solid-phase extraction (SPE) methodology. The column combinations are PHE to ENV, ABN, and HOB each; and ENV, ABN, and HOB each to PHE.

*Presented by: Laura Deloso - P23* *(Undergraduate, Analytical Chemistry)*

**Mass Spectrometric Signal Intensity of Lipid Assemblies and Liposomes**

Lipid assemblies are used for various biomedical purposes. Of these assemblies are micelles and liposomes. Membrane lipids have a readiness to aggregate over time even if prepared below the critical micelle concentration (CMC) which poses difficulty with data collection. We aim to analyze lipid assemblies and free lipids prepared in native conditions over time with the intent to determine the extent of impact to signal intensity. Liposomes will be synthesized in-house and diluted below their CMC in 99:1 water: MeOH with ammonium acetate. Free lipids will be prepared in similar conditions. Sample ionization will be done using surface acoustic wave nebulization (SAWN) paired with atmospheric pressure chemical ionization (APCI). SAW disruption for 30 seconds will be done. It has been observed that there is higher signal intensity for liposomes than free lipids, both above and below CMC. This data can be used in the future for both liposome and free lipid research in native conditions.

*Presented by: Simeon Fagbodun - P30* *(Undergraduate, Analytical Chemistry)*

**FAIMS-MS Data Analysis Automation and Enhancement with R**

The open source statistical programming language R has been applied to mass spectrometry through freely available packages such as rawrr. That package was designed to allow large scale automation of mass spectrometer data files for proteomics purposes; however, there are benefits to using R for other types of mass spectrometry, such as easy access to the wide range of other packages and tools that have been developed for R. These include machine learning, peak detection, and data visualization tools. Here the existing rawrr package is used and adapted to automate the processing of FAIMS raw data, with the potential for applying machine learning to further analyze the refined data.

*Presented by: David Garbutt - P21* *(Undergraduate, Analytical Chemistry)*

**Development of a Novel Sub Picomolar Method for Microscale Thermophoresis**

Microscale thermophoresis (MST) is a method used to detect and analyze interactions between molecules. The rate at which fluorescently tagged molecules move away from an application of heat is affected by molecular size (differences suggesting that a binding event has occurred) or shape (differences suggesting that a conformation change has taken place). Current instrument detection limitations dictate that sample sizes smaller than one picomolar cannot be accurately measured because the ratio between fluorescently dyed molecules and analyte compounds is too large within a typical binding assay to be recorded by modern detection methods. However, there are multiple biological mechanisms in which interactions between enzymes and ligands are known to occur at sub picomolar levels. We present data verifying a new technique which leverages a competition assay to accurately estimate molecular interactions at extremely low analyte concentrations.

*Presented by: William Lawless - P31* *(Graduate, Analytical Chemistry)*

**Orbitrap mass spectrometry for the determination of stable isotopes in amino acids.**

When it comes to determining isotope enrichment, IRMS (or "isotope ratio mass spectrometry") has long been approved by analytical chemists to be a reliable method. However, this technique has some limitations since it tends to call for a large sample quantity as well as high concentrations. Therefore, Orbitrap MS was introduced and further explored in terms of its applications in the field of tracing stable isotope degradation. Orbitrap MS has been found to be able to replace IRMS as it not only requires less sample amount and concentration but also works well with crude extract.

*Presented by: Chau My Bao Le - P20* *(Undergraduate, Analytical Chemistry)*

**Comparison of Acid Based Digestion Preparation of Forensic Soil For ICP-OES**

This report documents the analysis of 3 different acid based digestion methods of preparing forensic soil samples for ICP-OES. The methods focused only on changing the acids used to digest while keeping everything else constant. The 3 methods were a single acid digestion using $HNO_3$, a double acid digestion using $HNO_3$ and HCl, and finally a triple acid method using $HNO_3$, HCl, and HF. Analytical microwave environment was then simulated using heat and sealed Teflon containers. This was all done to determine the optimal method for finding trace metals often present in the human body and therefore in forensic samples.

*Presented by: Jacob Light - P32* *(Undergraduate, Analytical Chemistry)*

**Characterization of Multi-Component Liposomes using Mass Spectrometry**

Liposomes are nano-sized, spherical vesicles comprised of one or more phospholipid bilayers. These vesicles are easily synthesized and customizable in composition and cargo. Liposomes can be used as drug-delivery vesicles for anticancer medications as well as models for extracellular vesicles like exosomes. Mass spectrometry (MS) provides a useful tool for qualitative and quantitative data of liposomes and their contents. We are incorporating phospholipids, sterols, and soluble proteins into these liposomes, while also studying the encapsulation efficiency. As we increase the complexity of these vesicles, we can optimize MS parameters in hopes of one day analyzing whole exosomes.

*Presented by: Philrosen Monfiston Sejour - P26* *(Undergraduate, Analytical Chemistry)*

**More efficient synthesis of pillar[5]arenes**

I will be working on more efficient synthesis of pillar[5]arenes, and more specifically, finding a way to obtain (propargyl)5-T-P[5] at a higher yield. Currently, methods are successful at yielding this conformation about 6.25% of the time based on this paper: Rim-Differentiated C5-Symmetric Tiara-Pillar[5]arenes. We will be using a molding that will build sequentially to result in all five isoG molecules facing up, which is the preferred conformation.

*Presented by: Lily Ozell - P24* *(Undergraduate, Analytical Chemistry)*

**Supramolecular Asymmetric Amine Catalysis**

Organocatalysis reactions were performed to obtain higher yields in Aldol reactions of a specific catalyst used in Supramolecular Asymmetric Amine Catalysis. The main objective of the research is the obtention of such catalyst to develop more catalysis reactions in order to obtain a purer compound as a drug.

*Presented by: Rosabell Vega Ramirez - P27* *(Undergraduate, Analytical Chemistry)*

**Comparing Protein Precipitation (PPT) and Solid Phase Extraction (SPE) for novel fentanyl analog screening by LC-QTOF.**

Fentanyl is a synthetic opioid that is more than 50 times more potent than morphine and has many medical uses. Unfortunately, the opioid is also known to be responsible for thousands of overdoses and deaths every year in the United States. This is due to an illegal market that has been growing year by year for illegally produced fentanyl. This market has attracted rouge chemists to the illegal production of the drug and in turn the production of many fentanyl analogs that can be much stronger than their original form. These analogs can be difficult to identify in forensic labs with current screening methods. New methods need to be developed in order for the analogs to be detected. The method we are demonstrating is solid phase extraction (SPE) which will be compared to Protein Precipitation (PPT) before using LC-QTOF for final determination. We will be determining the LOD from a representative sample of analogs and comparing it to that of PPT.

*Presented by: Nickolas Schoenberger - P25* *(Undergraduate, Analytical Chemistry)*

**Using an open split interface to incorporate an laser cavity ring down spectrometer into a flow-through pyrolysis instrument to measure the 13C to 12C isotope ratio**

The carbon dating of sediment deposited under the Antarctic ice sheets for a long period of time was done by taking bulk carbon dates which average a samples age, using a flow-through pyrolysis instrument created in the lab we can separate the CO2 from the water and other unwanted molecules. This is then concentrated and measures with an accelerator or isotope ratio mass spectrometer to determine the 14C : 12C ratio and using that to determine the age of the sediment. We will be attempting to integrate a laser cavity ring down spectrometer into this instrument through an open split interface due to the small amount of flow in the current instrument and the much larger flow that the spectrometer needs to get an accurate measurement. This will allow us to measure not only the 14C : 12C ratio but also the 13C : 12C ratio which will help us determine which source of carbon is contributing to our samples.

*Presented by: Klayton Smith - P22* *(Undergraduate, Analytical Chemistry)*

**Testing for Bio-activity of Cladosporium cladosporioides and Emericellopsis alkaline and Subsequent Identification of Novel Compounds**

This project details the extraction, purification, and testing of two deep-sea fungal samples. Several goals bookmark this project, identifying bioactivity, isolating novel compounds, and structural predictions. Testing and identification are done with the use of a medium-pressure liquid chromatography system and several in-silico programs. The identified compounds are either classified as bioactive or non-bioactive and are pursed accordingly. By the end of the project we hope to find a novel compound bioactive against either Candida or ESKAPE.

*Presented by: Ashlyn Renee Bartley - P46* *(Undergraduate, Biochemistry)*

**Cadmium regulates NLRP3 inflammasome in RAW 264.7 murine macrophage**

Cadmium (Cd) is an environmental pollutant known to induce toxicity in the kidneys, heart, and lungs. The current antioxidant therapies for Cd toxicity such as chelation therapy pose safety and efficacy concerns. A better mechanistic understanding of how Cd alters the biochemical pathways that lead to inflammation and cell death is needed. Cytotoxicity was assessed to determine experimental doses of CdCl2. RAW cells were exposed to varying concentrations of CdCl2 (5uM, 10uM, 15uM) for 24 hours. Expression of NLRP3, Caspase-1, and apoptosis-associated speck-like protein (ASC) were assessed using Western Blot. Concentrations of IL-1$\beta$ and IL-13 in cell lysates were measured using ELISA kit. Approximately 50% cell viability occurs at 25uM Cd. NLRP3 inflammasome components were expressed more in Cd-treated cells compared to controls and showed higher concentrations of cytokines. The data suggest that Cd severely disrupts the biochemical homeostasis of macrophage cells.

*Presented by: Samuel Camilli - P56* *(Undergraduate, Biochemistry)*

**Novel synthetic ligands for the research of hydrogen bond templated construction of supramolecular nanostructures**

The frontier of a lot of research has been nanotechnology to construct novel structures and with a reasonable design, have properties that are functional with materials that can further be developed. Supramolecular chemistry is applied broadly in different scientific fields, this aids in building structures that can be applied in various facets of chemistry. Through the synthesis of different ligands of different importance, there will be an application of hydrogen bond template synthesis of helical nanofibers. The synthesis and the characterization of the supramolecular nanostructures will be presented as well as the application for further ongoing research.

*Presented by: Kerry Darelus - P51* *(Undergraduate, Biochemistry)*

**Discovery of a non-nucleotide small molecule inhibitor of STING and application in systemic lupus erythematosus**

There has been a steady rise noted in prevalence of antinuclear antibodies, a common hallmark of autoimmunity. SLE is an autoimmune disease that affects anywhere from 20 to 150 individuals per 100,000 people in the United States. There have been only two entries on the SLE

drug market in over 60 years. Nucleic acid sensors raised special attention among all the potential factors driving SLE pathogenesis. Detection of cytosolic DNA is largely through cGAS that functions upstream of STING protein. Activation of the cGAS-STING pathway results in induction of an innate arm of the immune system.

*Presented by: Mansi Gopu - P53* *(Undergraduate, Biochemistry)*

**Arylalkylamine N-Acyltransferase (AANAT) as Potential Insecticide Targets**

Arylalkylamine N-Acyltransferase (AANAT) catalyzes the transacylation from acetyl-CoA to arylalkylamines. In humans, this enzyme marks the penultimate enzyme in the melatonin biosynthetic pathway from serotonin. AANATs play a vital role in insects by inactivating neurotransmitters and contributing to the sclerotization of insect exoskeletons. AANATs are present in all organisms and aid in the completion of similar pathways. They are species specific, meaning that no two species have the same AANAT composition. The combination of its unique contribution to the formation of insect's exoskeletons and its species specificity make AANAT's of particular interest as targets for inhibition, and thus, insecticides.

*Presented by: Gabrielle Henry - P48* *(Undergraduate, Biochemistry)*

**Investigation of 4-arm and 8-arm lipid peptidomimetics as new antibacterial compounds.**

The research project will consist of conducting a synthesis of a 4-arm and 8-arm lipid peptidomimetic through the use of several amino acid building blocks within the peptide. This will be done through solid-phase peptide synthesis (SPPS) which is done throughout the lab to synthesize peptides containing multiple amino acids along the peptide. For now I am trying to synthesize this peptide with lysine as the starting amino acid building block but as verification and successful synthesis has been achieved on this peptide other building blocks will be incorporated such as arginine, serine, asparagine, valine, etc.

*Presented by: Jason R. Labayne - P50* *(Undergraduate, Biochemistry)*

**Metabolite Extraction, Purification, and Bioassay Analysis from Endophytic Fungi**

Deep-sea fungi can lead to novel discoveries in drug discovery due to the environmental barriers preventing research. This poster analyzes the secondary metabolites of a mangrove endophytic fungus to discover any antibiotic activity. Finding a high percentage of inhibition in the samples can lead to research for potential drugs from these samples. To do this, the fungi was grown in a rice bag for 21 days, separated through a separatory funnel, and ran through MPLC to create fractions. The fractions are analyzed by bioassay to find their antibiotic potential. P NMR and LCMS QTOF are used to identify what metabolites are causing said potential. MPLC showed high absorbances in the D-F fractions along the 254 and 280 nm wavelengths. Once the bioassay results arrive, I will be interested in the D-F fractions to see if the peaks match high

inhibition percentages in the bioassay. A bioassay result with 80% or higher inhibition means it's an important metabolite to study for drug discovery.

*Presented by: Sebastian Uribe Leon - P57* *(Undergraduate, Biochemistry)*

**Design of helical sulfono-$\gamma$-AApeptide targeting LC3B (ATG8)**

Autophagy is a cellular pathways that is responsible for the degradation of molecules such as pathogens, destructed organelles and macromolecules by delivering them to lysosome. To engulf the degraded molecules, a double-membraned autophagosome is formed by the help of receptors such as P62 in order to breakdown the molecules. A standard marker for autophagosomes is LC3-II therefore the quantification of LC3-II degradation could be used as a great indicator for autophagy. During autophagy, pro LC3 is converted to LC3-I which undergoes lipidation and get converted to LC3-II which is then degraded.Our synthesized foldamer (JC-6) is ought to inhibit the autophagy pathway and thus blocks the LC3-II degradation. To confirm this finding we have performed several experiments such as cell viability as assays which proved that our foldamer is cell permeable and disrupts the protein-protein interactions. We also carried out several imaging experiments, for measuring autophagic flux rate.

*Presented by: Mentalla Mahmoud - P54* *(Graduate, Biochemistry)*

**Binding Based Proteomic Profiling (BBPP) using Fatty acid amide analogs**

The role of fatty acid amides (FAAs) as cell signaling lipid has been validated by the discovery and investigation on endogenous FAAs. However, not many studies have been done on FAA and there is still a lot to learn. To investigate the roles of some of the FAAs, we have employed a strategy involving synthesis and characterization of FAA-targeted BBPP probe with photoreactive diazirine group and a clickable alkyne handle, and its use in labelling, identification, and validation of FAA binding proteins in Drosophila melanogaster. UV irradiation induces the formation of carbene in the diazirene that forms a covalent bond between the probe and the protein to which it is bound, thus allowing selective labelling of the proteome. The terminal alkyne is used in a click reaction to facilitate for fluorescent tagging, or biotin tagging for verification of labelling.

*Presented by: Imani McCalla - P49* *(Graduate, Biochemistry)*

**Toxic metal exposure and potential treatment of isolated mitochondria from Persea americana**

This study investigates the effects of toxic metals on mitochondrial respiration isolated from avocado tissues. Mitochondria were isolated from avocado tissues and exposed to varying concentrations of toxic metals, including zinc, lead, and silver. The respiratory activities of these isolated mitochondria were then measured using a redox sensitive dye. Our results demonstrated that toxic metals had a significant impact on mitochondrial respiration, leading to a dose-dependent decrease in oxygen consumption rates. Zinc and Lead were found to be the

most toxic, causing a significant inhibition of the electron transport chain, while silver had a less pronounced effect. These findings suggest that exposure to toxic metals can cause mitochondrial dysfunction, which may lead to cellular damage and disease development.

*Presented by: Devin McCollum - P61* *(Undergraduate, Biochemistry)*

**Synthesis of alternative $\alpha$-helix hybrids involving sulfono-$\gamma$-AApeptides**

Peptidomimetics is important for the development of biochemical and biomedical breakthroughs, but its stability in certain environments and solvents proves to be a difficulty in this field of study. For instance, semaglutide is a commonly known treatment for type-2 diabetes, but has many side effects and can be difficult to synthesize. Luckily, a certain drug discovery branch of Scripps Research called "Calibr", with the help of the University of South Florida Chemistry Department, develops an $\alpha$-helix that comprises of a hybrid of Sulfono-$\gamma$-AApeptide and GLP-1 that may potentially serve as a viable alternative to semaglutide. We will attempt to discover a mimetic of that hybrid that may serve additional medicinal purposes.

*Presented by: Vincent Khanh Nguyen - P58* *(Undergraduate, Biochemistry)*

**Atypical Protein Kinase C inhibitors abrogate malignant breast cancer**

This project focuses on utilizing aPKC inhibitor, ICA-1S (5-amino-1-((1R,2S,3S,4R)-2,3-dihydroxy-4-methylcyclopentyl)-1H-imidazole-4-carboxamide on a malignant breast cancer cell line, BT549 to observe the effect on cell proliferation and apoptosis. For both cell proliferation and apoptosis cells were treated with ICA-1S for 120 hours (5 days). Cell proliferation results show that ICA-1S (10uM) causes a 54% reduction for BT549 cell line. Additionally, it was observed by western blotting that ICA-1S induces apoptosis in BT549 cell line by showing an increase in the cleavage of caspase 3 and PARP. In addition, treatment with ICA-1S (10uM) for BT549 cells has caused a 50.2% decrease in the levels of PKC-, and also caused a 50.8% reduction of the phosphorylation of c-Jun. Previous studies has shown a co-relation between PKC- and c-Jun. Hence, further investigation will be conducted to find a signaling pathway involving the effect of ICA-1S on the correlation of c-jun and PKC-.

*Presented by: Nuzhat Oishee - P55* *(Graduate, Biochemistry)*

**Synthesis the building block for AA peptide**

AA peptide has been shown to have the potential ability against some diseases, it acts as the permeate cell membrane and binds to HIV's RNA, and potential use as a molecular probe to intervene in Alzheimer's disease. In order to synthesize the AA peptide, the building block of AA peptide is required and fundamental, the building block is stable and it can prepare for a long time use, therefore, synthesis of the building block is very important for the AA peptide use in disease. In my presentation, I will demonstrate the way to synthesize the building block for AA peptides.

*Presented by: Jun Ou - P60* *(Undergraduate, Biochemistry)*

**An In Silico Comparative Study of Interspecies Variability in Neurotransmitter Ligand-Receptor Interactions**

Research has shown that epigenetic regulation and spatial distribution of neurotransmitter receptors is linked to the expression of a variety of social behaviors and neurodevelopmental disorders. Studies on relevant receptor neurobiology have focused on signaling patterns as a therapeutic basis and have been successful in modulating behavior in several model organisms. Structure-based approaches may offer insight to molecular mechanisms contributing to observed irregularities in social behavior across species and contribute further investigation of neural circuitry. We examined receptors for dopamine (DRD1 and DRD2), oxytocin (OXTR1), and vasopressin (AVPR1) from a wide array of phylogenies totaling 465 proteins and conducted molecular docking with their respective ligand to compare binding affinity and other interactions. We highlight how this study contributes to our understanding of the role of receptor structure in broader neurobiological mechanisms and possible novel therapies.

*Presented by: Lalith Roopesh - P52* *(Undergraduate, Biochemistry)*

**Loss of endothelial derived laminin y1 exacerbates blood brain barrier disruption**

In this study, we generated laminin Y1 conditional knockout mice using Tie-2 Cre+ (Y1-TKO) that is known to express both endothelial and hematopoietic derived laminin. In this mechanistic study, we have shown that Y1-TKO mice have no change in tight junction expression, greater transcytotic activation, and greater exacerbation of blood brain barrier (BBB) disruption compared to normal mice. In addition, we have shown that endothelial, and not hematopoietic derived laminin, is the major contributor to this phenotypic change using bone marrow transplantation. These findings also suggest that endothelial derived laminin y1 plays a beneficial and crucial function in maintaining the blood brain barrier opening the doors for new therapeutic research.

*Presented by: Bilal Syed - P47* *(Undergraduate, Biochemistry)*

**A novel cyclic $\gamma$-AApeptide-based long-acting pan-coronavirus fusion inhibitor**

COVID-19 caused by SARS-CoV-2 and its variants has been posing serious threats to the global public health and economic stability, thus calling for the development of novel antivirals to combat the pandemic. Most of current therapeutic approaches generally lack broad-spectrum activity and exhibited much inferior activity toward emerging subtypes. Peptide pan-inhibitors targeting membrane fusion have demonstrated potent and broad-spectrum activity, however, their development is still hampered by their intrinsic enzymatic instability and low bioavailability. To this end, we employed the one-bead-two-compound (OBTC) cyclic $\gamma$-AApeptide library to screen against the Spike (S) protein of SARS-CoV-2 and discovered a series of macrocyclic peptidomimetics that showed promising antiviral activity.

*Presented by: Lei Wang - P59* *(Graduate, Biochemistry)*

**Peripheral and Central Auditory Function in a Mouse Model of Alzheimer's Disease**

Alzheimer's Disease (AD) is a form of dementia that is characterized by mental deterioration and can be detected through several changes occurring in the brain, such as the appearance of beta-amyloid plaques. In this study, we investigate peripheral and central auditory function in 5xFAD mice, which express human APP and PSEN1 transgenes with 5 AD-linked mutations. We used the auditory brainstem response (ABR) to assess hearing sensitivity and brainstem function. The ABR was used to determine the hearing thresholds at 5 different frequencies: 8, 12, 16, 24, 32 kHz, with the level of the tone ranging from 85 to 10 dB SPL. A loss of auditory nerve output, depressed auditory midbrain response, and an increase in thresholds on ABR audiograms (especially in the higher frequencies) were observed as time progressed. These results indicate that this AD mouse model is similar to many AD patients with hearing loss and may provide insight into deficits in auditory processing observed in AD.

*Presented by: Andrea Weitoschova - P46* *(Undergraduate, Biochemistry)*

**Identifying the Molecular Conformations of the Natural State of Branched Polyethylenimine: A Computational Query**

Computational modeling was sought out for conformational structure inferences upon the economic, biodegradable polymer, polyethylenimine as a single unit and a branched structure to understand the changes resulting from the processes of fabricating a drug containing the polymer, beginning with the molecule in an amorphous state dissolved in chloroform ($CHCl_3$).

*Presented by: Brandi Cook - P19* *(Graduate, Chemistry Education)*

**How students use properties to describe nucleophilic attacks**

The purpose of this study is to answer the question of how students use properties to describe nucleophilic attacks. Second semester organic chemistry students were asked to describe the first step in the mechanism of the reaction that would occur if the two given compounds, benzoyl chloride and ethyl amine, interacted. The students' open-ended responses were analyzed with deductive followed by inductive coding. Codes were grouped together by how they related to students' descriptions of nucleophilic attacks; for example, the codes describing compounds with "positive charges" and "negative charges" were grouped into an "opposites attract" code. Research on students' understanding of organic chemistry concepts and their ability to convey this understanding can assist in creating more efficient and effective teaching methods.

*Presented by: Nia Martin - P18* *(Undergraduate, Chemistry Education)*

**Synthesis of Antimicrobial Hybrid Organic-Inorganic Perovskite**

Perovskite semiconductors are one of the most versatile inorganic materials with applications in numerous fields. This research aimed to use specifically halide perovskites, to explore a previously untapped field: antimicrobial activity. When targeting such a property, novel syntheses with lead paired with existing organic drugs to modify the structure, may further optimize the

properties of the materials. Crystals were synthesized via a scalable hydrothermal synthesis method using organic linkers, then characterized using techniques such as X-ray Diffraction, Raman, photoluminescence spectroscopy, and thermogravimetric analysis. The synthesized materials are compatible for a wide variety of both traditional perovskite applications (i.e., gas sensing and solar cells).

*Presented by: Brianna Pecourt - P35* *(Undergraduate, Inorganic Chemistry)*

**Development of Phosphonium Based Metal Halide Perovskites**

Hybrid Organic-Inorganic Perovskites (HOIPs) is a class of metal halide materials that exhibit unique properties that enables them to be the next generation of semiconductor photovoltaic devices. Although HOIP semiconductors performance is comparable to already existing semiconductor devices, they still have some drawbacks and challenges that need to be addressed, such as low thermal stability, limited charge transport, and low mechanical stability. In this work we report the synthesis and characteristics of six new metal halide perovskite structures based on phosphonium organic spacers acting as structure directing agents. Their presence can enhance the thermal and mechanical stability. The reaction of Pb(II) with the phosphonium linkers in acidic media gave rise to 1D metal halide materials, consisting of chains of lead halide metal clusters.

*Presented by: Amanda Reyes - P36* *(Undergraduate, Inorganic Chemistry)*

**Chiral Metal Halide Semiconductors**

The importance of metal halide chemistry has been extremely prominent in our world. This is shown in our current day to day use within the technological conveniences we utilize such as street lamps and aides for photo development. These modern conveniences we have are due to the extreme versatility and wide range of properties these materials possess. One category of metal halides is that of halide perovskites. Perovskites have shown time and time again that they are an invaluable class of material due to applications pertaining to solid state solar cells with a greater efficiency than current commercial solar panels. However, these compounds are expected to be promising for applications beyond photovoltaics, such as Circular Polarized Light photonics and spintronics. In this work, we utilized chiral organic linkers (S), for the synthesis of two new chiral materials (S-L)$SbBr_5$ and (R-L)$SbBr_5$ for further research into these promising yet unexplored facets of perovskite materials.

*Presented by: Brandon Sauval - P33* *(Undergraduate, Inorganic Chemistry)*

**Synthesis of Hybrid Metal Halides for Biomedical Applications**

Hybrid organic-inorganic metal halides are semiconductors known for their unique optoelectronic properties. These materials are utilized efficiently for a plethora of applications, such as solar cells, LEDs, photocatalysis and photodetection. Our work focuses on a less explored direction, that is the synthesis of biocompatible metal halides, while maintaining the photoelectric performance of fully inorganic metal halide and perovskite compounds. In this project we tailor the

optoelectronic properties of these materials for biomedical applications. To accomplish this, we synthesize compounds that are water stable and have good photostability. We have acquired new materials based on nontoxic metals such as bismuth and antimony. Upon extensive structural and optical characterization, we will evaluate the new semiconductors towards applications such as photodynamic-therapies and antimicrobial medications.

*Presented by: Sarah Troutt - P34* *(Undergraduate, Inorganic Chemistry)*

**Synthesis and optimization of the Piancatelli Rearrangement in search of new antiviral drug implication**

The Piancatelli Rearrangement is utilized in the synthesis toward applications in therapeutic treatment, as well as potential drug research discovery by converting furanyl alcohols into 4-alkoxy or 4-hydroxycyclopentenones. In this work we are pursuing a novel variation of this rearrangement that will allow for carbon-based substitution at the 4 position. This could be used toward new antiviral drugs, as well as being seen as furthering the important significance of the rearrangement in the research industry as well as the application in therapy. Results to date will be presented.

*Presented by: Kaylee Barnhill - P8* *(Undergraduate, Organic Chemistry)*

**Synthesis of Various Structural Analogs of Efavirenz**

Cyclopropylacetylene (CA) is a key intermediate in the synthesis for the Human Immunodeficiency Virus (HIV) reverse transcriptase inhibitor, Efavirenz (EFV), an antiviral drug used to treat HIV. CA is an expensive raw material, difficult to obtain, employed in the preparation of medications to combat Acquired Immunodeficiency Syndrome (AIDS). It was found that the yield could be enhanced by the utilization of PCl5; however, this resulted in unwanted ring openings. To address this issue, a one pot synthesis was employed using Ph3PCl2 as a mild chlorinating agent. In addition, a new analog has been proposed substituting the cyclopropyl group for alternative hydrocarbons. Instead of using a cyclopropyl ring, a larger ring with more than three carbons can result in less ring strain; therefore, less ring opening. Previous experiments have tested other ring structures; however, larger cyclic hydrocarbons have yet to be studied within these conditions.

*Presented by: Elizabeth Sanchez Bautista - P4* *(Undergraduate, Organic Chemistry)*

**Drug discovery of Novel Bioactive Compounds against different Strains of Candida**

Candidiasis is an infection caused mainly by a Candida fungus. It affects mainly the gastrointestinal tract, mostly mucosal and along the skin of the body. A disturbing 30-40% of these infections result in ultimate death. Majority of susceptible patients are people with impaired immune system as over 90,000 people in the United State contracted this infection in a year1. Endophytic fungus are naturally micro-organisms that colonize the inter and intracellular tissue spaces of host and provide beneficial advantages to its host through the secretion of metabolites2.

These metabolites are potential drug candidates. C. auris and C. albicans are multidrug-resistant against certain classes of antifungals3.This research project seeks to generate active secondary metabolites from endophytic fungus. Fungal extracts will be concurrently subjected to bioassay and nuclear magnetic resonance (NMR) spectroscopy guided approaches to aid in the search for compounds with Candida activity.

*Presented by: Sylvester Osei Bobbie - P17* *(Graduate, Organic Chemistry)*

**On the Synthesis and Reactivity of Amino Alcohols as Chiral Templates for Building Blocks in Peptidomimetic Synthesis**

$\beta$-Amino-alcohols derived from natural amino acids have been used extensively as a powerful source of chirality. In fact, they are present naturally occurring and pharmacologically active molecules, and the relative stereochemistry of the hydroxy and amino groups is highly important for biological activity. In our laboratories, $\beta$-Amino alcohols and their derivatives have played seminal roles as building blocks in peptidomimetic synthesis. With this goal in mind, the formation of chiral amino alcohols was accomplished by the reduction of -amino acids using $NaBH_4$-$I_2$ in anhydrous THF. Using this procedure, no racemization of the chiral center was detected. In turn, protection of the primary amine using benzyl bromide in acetonitrile produced the N,N-Dibenzylamino alcohols, respectively. Subsequently, the alcohols were smoothly converted to the desired bromide in high yield by reacting with $SOBr_2$ and DMF. The product was spectroscopically pure, and no further purification was necessary.

*Presented by: Emma Cartwright - P5* *(Undergraduate, Organic Chemistry)*

**Analysis of the secondary metabolites of various species of bacteria collected from Antartica**

Secondary metabolites are becoming a new area of interest for developing novel antibiotics to treat antibiotic resistant pathogens. Samples of Sporosarcina psychrophile, Sporosarcina saromensis, Sporosarcina terrae, Sporosarcina siberiensis, Sporosarcina ureae, Nitratireductor aquibiodomus, Nitratireductor pacificus, Dietzia maris, Arthrobacter stackerbrandtii, Agrococcus jenensis collected from the oceanic sediment in Antarctica were cultured to 1 liter stock solutions. The bacteria and the supernatant were separated using the centrifuge. The supernatant was analyzed using mass spectrometry and NMR. The bacteria cells were lysed, and the metabolites were extracted using ethyl acetate. The metabolites were analyzed with mass spectrometry and NMR.

*Presented by: Bonnie Foust - P3* *(Undergraduate, Organic Chemistry)*

**Synthesis of Peptidomimetics as Potential Anticancer Agents and Biomedical Applications**

Numerous physiological and pathological stimuli induced programmed cell death (apoptosis), and the Bcl-2 family of oncoproteins plays a central role in this regulation. Proteins such as Bcl-2 are known to inhibit apoptosis, and 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.

*Presented by: Ashley Graham - P2* *(Undergraduate, Organic Chemistry)*

**Synthesis and optimization of the Piancatelli Rearrangement in search of new antiviral drug implication**

The Piancatelli Rearrangement is utilized in the synthesis toward applications in therapeutic treatment, as well as potential drug research discovery by converting furanyl alcohols into 4-alkoxy or 4-hydoxycyclopentenones. In this work we are pursuing a novel variation of this rearrangement that will allow for carbon-based substitution at the 4 position. This could be used toward new antiviral drugs, as well as being seen as furthering the important significance of the rearrangement in the research industry as well as the application in therapy. Results to date will be presented.

*Presented by: Jessica Heintz - P7* *(Undergraduate, Organic Chemistry)*

**Utilization of Cannabinoids as Molecular Probes: Furthering Our Understanding of The Endocannabinoid System**

Tetrahydrocannabinol (THC) and cannabidiol (CBD) have been shown to reduce amyloid plaques, one of the causes of Alzheimer's disease (AD). To explore this, we can synthesize novel labeled cannabinoids. These cannabinoids can be used as well as other analogs to probe the endocannabinoid system, specifically in AD mice. This experiment can help identify potential therapeutics for the prevention of AD.

*Presented by: Kerwin Jaropillo - P9* *(Undergraduate, Organic Chemistry)*

**One-Bead-Two-Compound Macrocyclic $\gamma$-AApeptides Screening Library Against ADRB2**

Combinatorial Library Synthesis refers to the method of creating a large number of diverse chemical compounds in a single synthesis reaction. This method involves the simultaneous preparation of a large number of compounds by mixing starting materials in various combinations. This approach is used to synthesize and screen large collections of compounds in a high-throughput manner to identify new compounds with desired properties. My research project is based on the concept of combinatorial library synthesis to develop a cyclic peptidomimetic ligands library for targeting proteins. In order to achieve that, we developed an unprecedented one-bead-two-compound (OBTC) combinatorial library based on a novel class of macrocyclic peptidomimetics

$\gamma$-AApeptides. In this combinatorial library, we utilized Dde-protected $\gamma$-amino acids for the coding region, and macrocyclic $\gamma$-AApeptides employed by thioether linkage for functional ligand region as OBTC for screening against protein targets.

*Presented by: Sihao Li - P15* *(Graduate, Organic Chemistry)*

**Developing Peptidomimetic Scaffolds as Potential Therapeutics in Clinical Chemotherapy**

Numerous physiological and pathological stimuli induce programmed cell death (apoptosis), and the Bcl-2 family of oncoproteins plays a central role in this regulation. Proteins such as Bcl-2 are known to inhibit apoptosis, and 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 carbazate and dithiocarbazate peptidomimetics, respectively. This study is now being extended to the synthesis of other de novo analogs. Utilizing our aforementioned protocols, various scaffoldings are being employed for the development of novel artificial biomolecules, which may result in biological behaviors regarding the disruption of protein-protein interactions and may serve as potential therapeutics in clinical chemotherapy.

*Presented by: Robert Logue - P13* *(Undergraduate, Organic Chemistry)*

**Isolation of indole diterpene class compound from mangrove endophytic fungus: HM13-24C-E1**

A vast yet less persuasive source of interesting chemistry consists of marine ecology and mangrove areas. To assuring the most usage of these sources, a mangrove endophytic fungus: HM13-24C-E1 was collected, cultured, and purified to identify compounds responsible for the bioactivity against ESKAPE pathogens. Secondary metabolites of the mangrove endophytic fungi HM13-24C-E1, collected from Florida, were isolated and characterized using dereplication and compound isolation methods. Methods of dereplication using LC-MS/MS applied to the fungi resulted in the identification of known toxins and diverse secondary metabolites using molecular networking (GNPS). Isolated compounds were prioritized and characterized using NMR analysis and mass spectrometry techniques. As a result of the employment of these techniques, a bioactive Indole Diterpene against the ESKAPE pathogens was isolated and characterized.

*Presented by: Sefat Munjerin - P14* *(Graduate, Organic Chemistry)*

**Synthesis and optimization of the Piancatelli Rearrangement in search of new antiviral drug implication**

The Piancatelli Rearrangement is utilized in the synthesis toward applications in therapeutic treatment, as well as potential drug research discovery by converting furanyl alcohols into 4-alkoxy or 4-hydroxycyclopentenones. In this work we are pursuing a novel variation of this

rearrangement that will allow for carbon-based substitution at the 4 position. This could be used toward new antiviral drugs, as well as being seen as furthering the important significance of the rearrangement in the research industry as well as the application in therapy. Results to date will be presented.

*Presented by: Nellie Onugha - P12* *(Undergraduate, Organic Chemistry)*

**Activity Based Probe for the Fatty Acid Amide System**

Fatty acid amides (FAA) are a type of endogenous signaling molecule that are of interest for creating medicine for a variety of diseases. Anandamide, the most notable ethanolamide, possesses analgesic and anti-inflammatory properties. Among the primary amides, oleamide is the most studied and is associated with sleep regulation. These compounds point to the benefits of understanding functions and biosynthesis of other fatty acid amides. Developing probes of fatty acid amides could provide insight to the proteins responsible for specific effects. This knowledge would allow for manipulation of the fatty acid amide system, leading to future medications to remedy pain and disease, which could address sleep disorders, pain management, and emotional regulation.

*Presented by: Keyla Gonzalez Ramirez - P10* *(Undergraduate, Organic Chemistry)*

**Identification of Novel Antibacterial and Antimitotic Agents from Fungal Extracts**

Microbial resistant to drugs is an ever-increasing threat. ESKAPE pathogens (Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter species, Pseudomonas aeruginosa, Enterobacter species) as well as C. Albicans and C. Auris cause a significant amount of antimicrobial resistant infections worldwide, and thus, the study of new antimicrobial agents that can be of use against these pathogens is of upmost necessity. Having millions of years of experience against microbes, Fungi are well equipped to battle microbes. They produce a wide array antibacterial and antimitotic agents that have been used in modern medicine ever since the 1930's with the discovery of penicillin from Alexander Fleming's studies. Emulating this, the study of several fungal species from Tapachula, Mexico was conducted in a bioassay driven manner, along with the use of liquid Chromatography techniques, Mass spectrometry and Nuclear Magnetic Resonance imaging.

*Presented by: Ezequiel Cruz Rosa - P6* *(Graduate, Organic Chemistry)*

**Chemical Profiling of Secondary Metabolites Isolated from Mangrove Endophytic Fungi**

Mangrove endophytic fungi holds secondary metabolites produced in response to the stressing ecosystem. After culturing and partitions, the sample was subjected to MPLC, in which 10 fractions were collected based off time. Fractions D and E, collected between 40-70% ethyl acetate, exhibit the most bioactivity against the ESKAPE pathogens, Candida albicans, Candida auris and Anti-Leishmaniasis. While both fractions D and E were submitted to normal phase HPLC,

fraction D was most active against K. pneumoniae, A. baumannii and Anti-Leishmaniasis while fraction E was active against four strains of Candida albicans (2786, 76458, 90029, and 28121) and one strain of Candida auris (0385). Penicillic acid was one of the secondary metabolites isolated from fraction D, which shows promising activity. Chemical profiling has been completed on the metabolites extracted, including 1H NMR, 13C NMR, LCMS-QTOF, GNPS, SIRIUS, ESKAPE, Candida albicans, Candida auris and Anti-Leishmaniasis.

*Presented by: Stephanie Paola Suarez - P16* *(Graduate, Organic Chemistry)*

**Synthesis and optimization of the Piancatelli Rearrangement in search of new antiviral drug implicatio**

The Piancatelli Rearrangement is utilized in the synthesis toward applications in therapeutic treatment, as well as potential drug research discovery by converting furanyl alcohols into 4-alkoxy or 4-hydroxycyclopentenones. In this work we are pursuing a novel variation of this rearrangement that will allow for carbon-based substitution at the 4 position. This could be used toward new antiviral drugs, as well as being seen as furthering the important significance of the rearrangement in the research industry as well as the application in therapy. Results to date will be presented.

*Presented by: Ariel Woods - P1* *(Undergraduate, Organic Chemistry)*

**Antimicrobial Guanidinylate polycarbonates with potent in vitro and orally in vivo activity against C. difficile**

The emerging antibiotic resistance has been named by World Health Organization (WHO) as one of the top 10 threats to public health. Among different strategies to combat these bacteria, host-defense peptide (HDP)- mimicking polymer materials are found versatile and promising in developing antibiotic biomaterials. However, a vast majority of antibiotic polymer applications were limited to the topical application due to their potential systematic toxicity. Herein, we report the design and synthesis of a series of new biodegradable lipidated antimicrobial guanidinylate amphiphilic polycarbonates. These polymers showed potent antimicrobial activities against both Gram-negative and Gram-positive bacteria with the rapid kinetic killing ability and and a low tendency to develop the resistance. More importantly, the optimal polymer showed significant antibacterial activity against C. difficile infection (CDI) in vivo via oral administration.

*Presented by: Menglin Xue - P11* *(Graduate, Organic Chemistry)*

**Investigating $CO_2$ Adsorption in GEFSIX-3-M and SFSIX-3-M (M = Co, Ni) Analogues**

GCMC simulations of CO2 adsorption for GEFSIX-3-M and SIFSIX-3-M (M=Co, Ni) were performed to investigate how substituting the inorganic pillars (GeF6 2- vs SiF6 2-) and saturated metals ($Ni_2$+ vs $CO_2$+) affect the $CO_2$ adsorption properties. These MOFs consist of a

2-dimentional square grid consisting of metal ions coordinating to Pyrazine ligands; the metal ions also pillar in the 3rd dimension using the inorganic anions. Classical force fields for all MOFs were developed; they include partial charges, the polarizability values, and Lennard-Jones potential parameters to model electrostatic, induction, and dispersion/repulsion interactions respectively. The simulations were performed at 273K and 298K and pressures up to 1 atm using 3 different models: TraPPE, PHAST, and PHAST*. The simulations in all 4 MOFs using all three models reveal a simulated CO2 uptake and isosteric heat of adsorption trend that is mostly consistent with that of experimental observations.

*Presented by: Pierce Asiatico - P43* *(Undergraduate, Physical Chemistry)*

**Photophysical Studies and Nitroaromatic Sensing Associated with the Porphyrinic Metal Organic Framework PCN-222**

Metal-Organic Frameworks (MOFs) are regularly nanoporous materials that have wide ranging applications including drug delivery, light harvesting, and sensing. The integration of light sensitive elements within MOFs, like porphyrins and metalloporphyrins, enable them to be used for optical sensing of a wide variety of analytes. Porphyrins can be incorporated within the MOF framework itself, serving as ligands connecting transition metal nodes, or as guests within the MOF cavities. The PCN-222 MOF is an example of a photoactive material in which tetrakis(4-carboxyphenyl)porphyrin (TCPP) is an integral component of the framework and acts as an optical sensing element. From the single crystal X-ray structure, we have determined TCPP to be highly distorted giving rise to perturbed photophysics including reduced excited state lifetimes and blue-shifted emission spectra. We also examined the effectiveness of the distorted TCPP in the PCN-222 framework to sense nitrobenzene via quenching.

*Presented by: Julia DeMatteo - P38* *(Graduate, Physical Chemistry)*

**Systematic Assessment of the Flexibility of DNA Containing $O_6$MeG Lesions Using MD Simulations**

DNA lesions which do not distort the overall helical structure can be recognized and excised by a suite of enzymes of the base excision repair (BER) pathway. The efficiency of these enzymes depends on the deformability of the DNA double helix, and deformability, in turn, depends on sequence context. Specifically, the nearest neighbor context, of which the tetranucleotide context is a minimal representation. Here we systematically assess the effect of the 6-O-methylguanine ($O_6$MeG) lesion on the flexibility of DNA by MD simulations. To increase statistics on each tetranucleotide motif, we simulated all 64 GX(OYZX)3G 15mer sequences, where X, Y, Z could be any of the bases A, C, G, T, and O equals either 6-O-methylguanine base paired to C, or G base paired to C as undamaged control. Base and step parameters were assessed, as well as persistence lengths. A comparison between sequences revealed how sequence context affects the mechanical deformability of O6MeG-damaged DNA.

*Presented by: Emmanuel Eni - P41* *(Graduate, Physical Chemistry)*

**Investigations of Cytochrome C and Myoglobin Protein Conformations upon Encapsulation into ZIF-8 and Tb-mesoMOF Frameworks**

Using the MOFs (Metal Organic Frameworks) ZIF-8 and Tb-mesoMOF, the proteins Cytochrome C and Myoglobin will be analyzed to determine the internal conformation upon entering the pores. It is theorized that the Investigations of Cytochrome C and Myoglobin Protein Conformations upon Encapsulation into ZIF-8 and Tb-mesoMOF Frameworks protein must partially unfold to enter into the MOF, as the size of the protein is too large to fit into the MOF in its native conformation. The MOF will be analyzed using UV-Vis and fluorescence data to determine if the proteins are in their native conformation or denatured within the MOF.

*Presented by: Dawson Lund - P42* *(Undergraduate, Physical Chemistry)*

**Investigating the Mechanisms of Uracil-Induced DNA Lesions in Different Sequences**

Cellular DNA is susceptible to many different types of damage, and a common daily lesion is the presence of uracil. Uracil results from either spontaneous deamination of cytosine or through misincorporation during the replication process. The presence of uracil is problematic due to its similarity in structure to thymine and can lead to mutations in the genome. DNA sequences were constructed in different motifs to study the role of nearest neighbors to the lesion. Sequences containing an AUA, AUT, TUT, and TUA context were studied. Simulations of unbiased damaged DNA exhibited bending and uracil base flipping. To further investigate this phenomenon, 2D umbrella sampling were used to study the free energy barriers related to bending and flipping. In certain sequence contexts, neighboring bases would interact with the complementary base of uracil, leading to a register shift.

*Presented by: William Rechkemer - P40* *(Undergraduate, Physical Chemistry)*

**Use of CAM Model to Predict Trends of Ozone and its Precursors**

In this research project the Community Atmosphere Model will be used to run a chemistry simulation of the atmosphere over a period of at least 35 years. A program will be rewritten that can calculate the trends of ozone and its precursors (NO2, CO, OH, etc).

*Presented by: Samuel Shriver - P37* *(Undergraduate, Physical Chemistry)*

**Investigating H2 adsorption among soc-MOF analogues using Grand Canonical Monte Carlo simulations**

Metal–organic frameworks (MOFs) are a class of hybrid materials that consist of organic ligands coordinated to inorganic clusters to produce highly porous, crystalline networks. Grand Canonical Monte Carlo (GCMC) simulations of H2 adsorption were carried out on three isostructural MOFs with square octahedral (soc) topology: In-soc-MOF-1a, In-soc-MOF-1b, and Fe-soc-MOF-1a. Overall, the results from this theoretical study showed how making small modifications to the soc-MOF structure (i.e., substituting the metal ion and counterion) resulted in varying

H2 adsorption properties. This could provide valuable insights into the rational design of new MOFs for improved H2 uptake in the quest for meeting commercial H2 storage targets.

*Presented by: Chloe Starkey - P44* *(Undergraduate, Physical Chemistry)*

**Calculation of Conformational Free energies of Z-DNA Using Confinement Method with AMBER OL15 Force Field**

Free energy differences are critical quantities to understanding the function of many biomolecules. The free energy difference between Z and B conformers of a DNA sequence is found using the confinement method and free energy perturbation. Dynamics are propagated using CHARMM with the AMBER OL15 forcefield. The confinement method simplifies the task of calculating Free energy differences greatly by not requiring a reaction coordinate. Free energy perturbation is employed to calculate desolvation free energies to complete the thermodynamic cycle between B and Z conformers. Unique to this paper was the use of the AMBER OL15 forcefield in CHARMM. The AMBER OL15 forcefield has shown significant improvement in the simulation of Z-DNA. To this end, ParmEd and in-house allow the OL15 parameters to be used with CHARMM. The results yield low error within chemical accuracy, and indicate a massive difference in free energy, which corresponded to the results achieved using the CHARMM36 forcefield.

*Presented by: Alvin Uppgard - P39* *(Undergraduate, Physical Chemistry)*

# Judges

**University of Virginia**

Marilyne Stains, Ph.D.

**Eckerd College**

George F. Riegel, Ph.D.

**Southeastern University**

Ralph Salvatore, Ph.D.
Louise Sideras, Ph.D.

**Keiser University**

Suchi Tiwari, Ph.D.

**University of California San Diego**

Fiona Kerns Ph.D.

**University of South Florida**

Laura Anderson, Ph.D.
Bill Baker, Ph.D.
Kirpal Bisht, Ph.D.
Jianfeng Cai, Ph.D.
Marlius Castillo, Ph.D.
Frankie Costanza, Ph.D.
Betul Demirdogen, Ph.D.
Kimberly Fields, Ph.D.
Wayne Guida, Ph.D.
Ushiri Kulatunga, Ph.D.
Jim Leahy, Ph.D.
Wenqi Liu, Ph.D.
Abdul Malik, Ph.D.
Anamika Mishra, Ph.D.
Tony Pham, Ph.D.
Chavdar Slavlov, Ph.D.
Ioannis Spanopoulos, Ph.D.
Christie Tang, Ph.D.

# Organizing Committee

**Sponsor(s)**
Tampa Bay ACS
Chemistry Council of Graduate Students

**Staff and Faculty Support**
Michael Abaskaron
Theresa Evans-Nguyen, Ph.D.
Kimberly Fields, Ph.D.
Sergio Garcia
Scott Lewis, Ph.D.
Joshue Martinez
Christina Nelson, Ph.D.
Chavdar Slavlov, Ph.D.

**Committee Members**
Alissa Anderson
Sarah Dietrick
Alexandra Keidel
Angelie Matar
Stephanie Suarez
Bobbie Sylvester
Jessica Young
Xue Zhao

**Committee Chairs**
Guy W. Dayhoff II
Ezequiel Rosa Cruz
Jennifer Williams