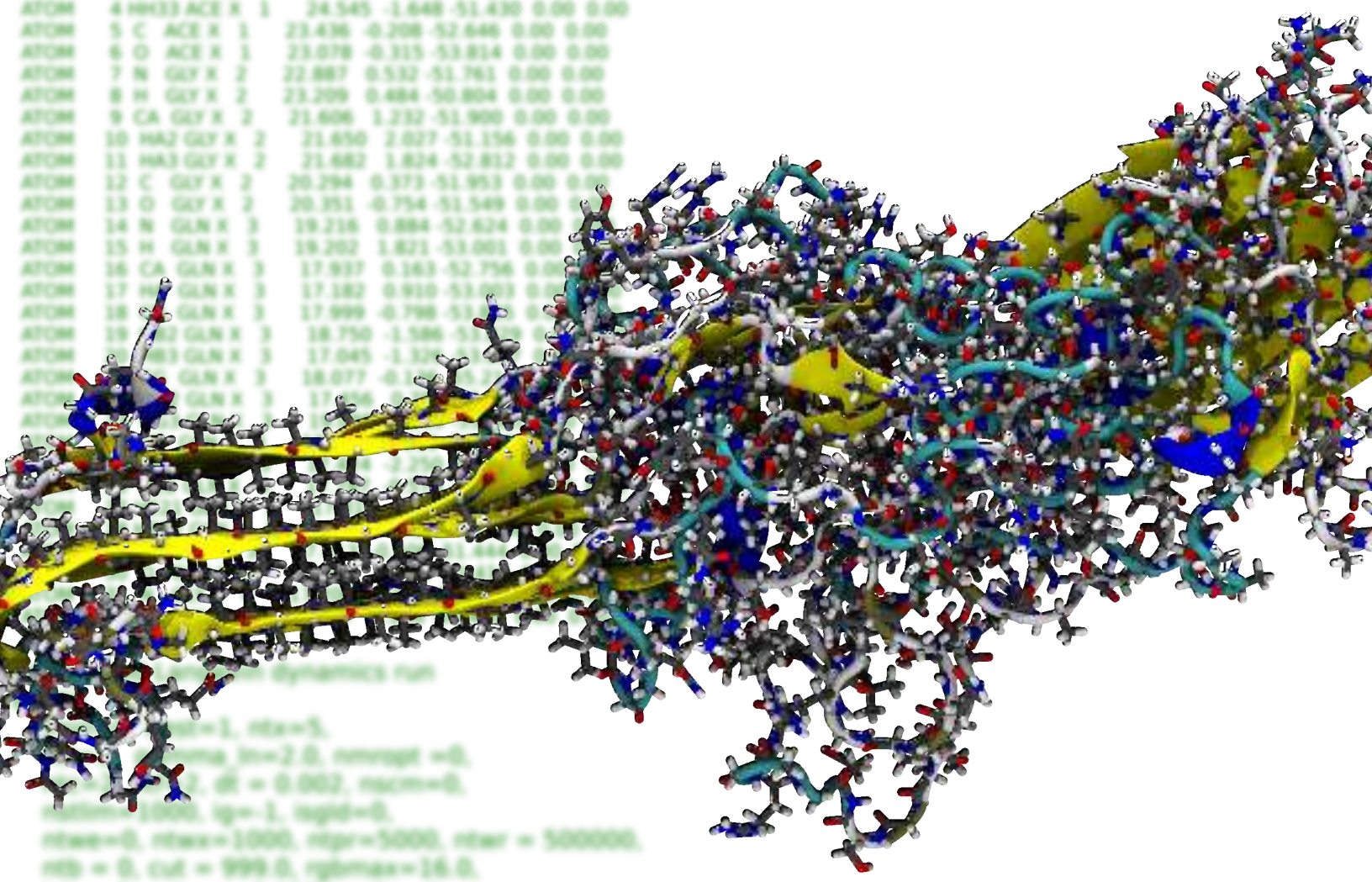
Raymond N. Castle
Student Research Conference

14th
April 2, 2016



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University of South Florida
Department of Chemistry
4202 East Fowler Ave., CHE205
Tampa, FL 33620

14th Raymond N. Castle Student Research Conference

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Welcome from the Castle Conference Committee

Dear Colleagues and Friends,

Welcome to the 14th Raymond N. Castle Student Research Conference hosted by the University of South Florida. In honor of Dr. Raymond N. Castle, this Conference was created to promote his goals of scientific collaboration and science education.

The Raymond N. Castle Student Research Conference continues to be organized by students for students as an excellent opportunity for undergraduate and graduate chemistry students to share scientific ideas and research progress. Students are encouraged to not only gain presentation experience, but to use the conference as a chance to further their research endeavors by gaining valuable feedback from other members of the chemistry community. It is this interaction and the sharing of ideas that makes the Raymond N. Castle Student Research Conference a worthwhile experience and a continued success.

We are especially proud of the research done by all students in the department, both graduate and undergraduate. With the continued success of the Raymond N. Castle Student Research Conference and to more clearly promote scientific collaboration, we have expanded our invitation for presentation to students in other Natural Science Departments as well as Colleges and Universities in Tampa and the surrounding areas. Today, we have an opportunity to hear from students in chemistry related disciplines from around Florida. Chemistry research will be highlighted with our special guest, Dr. Steven Castle. We encourage everyone to take advantage of this occasion and attend both the poster and oral presentations, especially the Plenary Lecture. We are honored and greatly appreciative that Dr. Castle will be giving a presentation on her exciting research and experience in the field of chemistry.

Lastly, we would like to thank all that chose to volunteer their time and efforts, particularly the judges, and Dr. Leahy for helping us plan and coordinate this year's conference. In addition, we are grateful for the financial support that allows us to host this conference and owe special thanks to Dean and Barbara Martin, Tampa Bay Local Section of the American Chemical Society, University of South Florida College of Arts and Sciences, and University of South Florida ResearchOne, as well as the multiple other sponsors and affiliates who have generously contributed to this event. Most importantly, this conference would not exist without the efforts of those of you presenting your research today. Therefore, we gratefully acknowledge you and your research advisors, as well as all in attendance. Thank you all and we hope you enjoy and learn from the 14th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

14th Raymond N. Castle Student Research Conference Committee

Committee Members

Darrell Cole Cerrato (Chair)
Alekhya Nimmagadda
Douglas Franz
Adam Hogan
Ankush Kanwar
Sri Krishna Nimmagadda
Zachary Schultz
Rebecca Vaclav

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Adam Hogan
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Specials Thanks

Kimberly Read
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14th Raymond N. Castle Student Research Judges

University of South Florida

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Brian Space
Dale Chaput
Daniel Cruz-Ramirez de Arellano
Edward Turos
Francois Villemot
Hyun Joo Kil
Jhon Figueroa
Jianfeng Cai
Jim Leahy
Ellen Leahy
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Laura Anderson
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Wayne Guida
William A Maza
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H. Lee Moffitt Cancer Center & Research Institute

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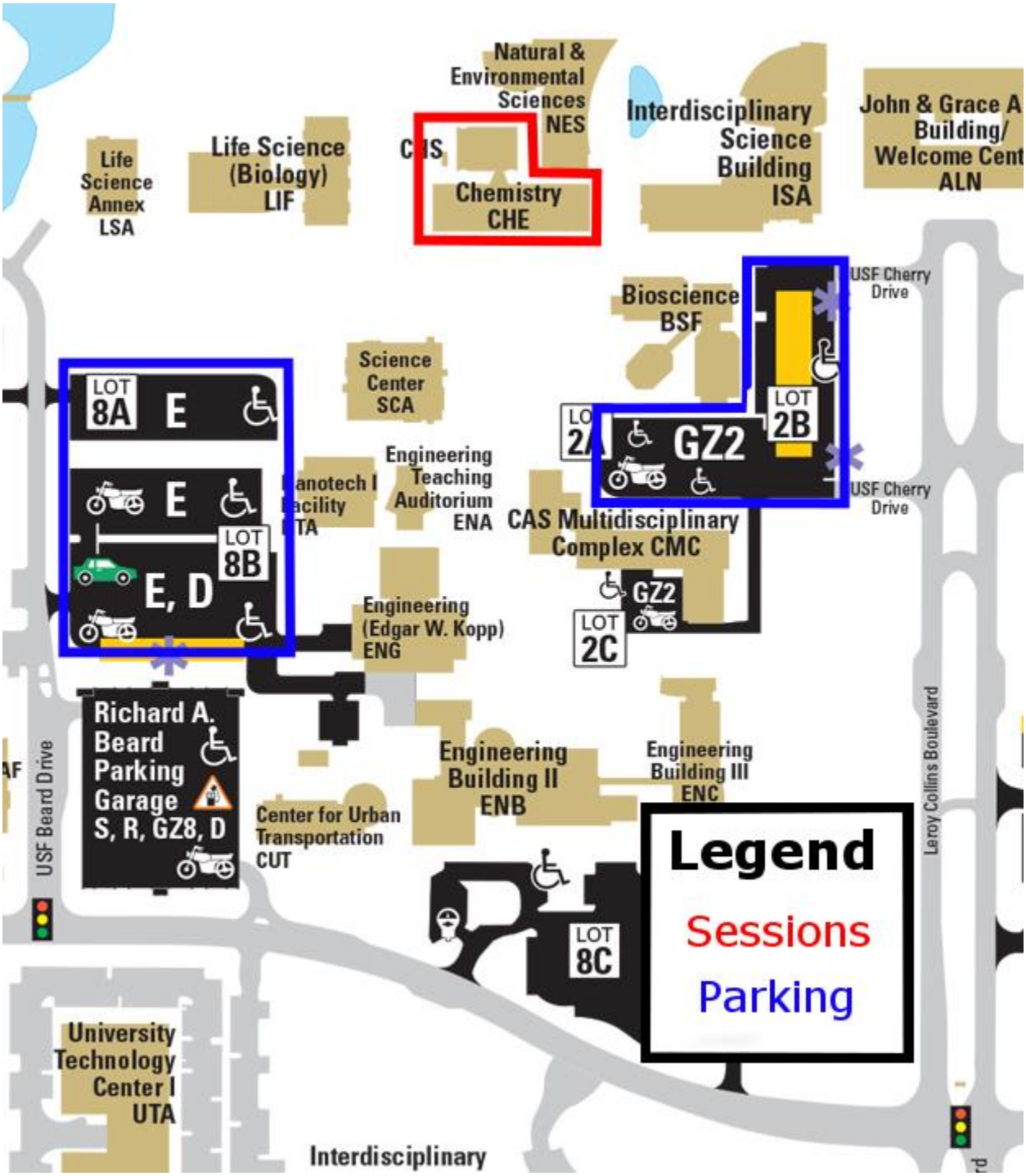
Paul Stewart, PhD

ACS Tampa Bay Local Section Members

Dan Pernazza, PhD
Sujeewa Ranatunga, PhD
Eric Johnson, PhD

Building Map



Schedule of Events

Saturday, April 2, 2016

8:00 AM	-	9:00 AM	**Welcome Session** - *Registration and Breakfast*	Chemistry Courtyard
9:00 AM	-	10:45 AM	**Morning Talk Session** *Graduate Student Presentations*	CHE 100
10:45 AM	-	11:00 AM	**Break**	
11:00 AM	-	11:15 AM	**Castle Conference Welcome**	CHE 100
11:15 AM	-	12:15 PM	**Plenary Speaker - Dr. Steven Castle**	CHE 100
12:15 PM	-	1:00 PM	**Lunch** *Sponsored by the ACS Tampa Bay Local Section*	Chemistry Courtyard
12:30 PM	-	1:00 PM	**ACS Tampa Bay Local Section General Body Meeting**	CHE 100
1:00 PM	-	3:00 PM	**Poster Session** *Graduate and Undergraduate Presentations*	CHE 1st Floor Classrooms
3:00 PM	-	3:15 PM	**Break**	
3:15 PM	-	5:00 PM	**Afternoon Talk Session** *Graduate Student Presentations*	CHE 100
5:00 PM	-	5:15 PM	**Break**	
5:15 PM	-	5:30 PM	**Awards Ceremony**	CHE 100

Save the Date for the 15th Raymond N. Castle Student Research Conference:
March 25th, 2017

Professor Raymond N. Castle

1916 – 1999

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.

Dr. Steven Castle

Plenary Speaker

The University of South Florida's Department of Chemistry is proud to be celebrating the 100th birthday of the conference founder, Dr. Raymond N. Castle, with his grandson, Dr. Steven Castle of Brigham Young University.

As honored guest and plenary speaker for this landmark occasion, Dr. Steven Castle will present his research:

New Strategies for the Synthesis of Unusual Peptides

The complex structures of peptide natural products provide inspiration for the development of new methods in synthetic organic chemistry. Additionally, the potent and selective bioactivity of many of these compounds provides opportunities to use organic synthesis to answer important questions in chemical biology. Both published and unpublished results from our ongoing synthesis of the anticancer peptide yaku'amide A will be presented. In addition, our efforts to use the methodology developed in this endeavor to construct other important biologically active peptides will be described.

Dr. Dean and Barbara Martin

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 attended 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 the coordination chemistry of natural water systems, including problems of red tide and aquatic weeds and they have collaborated in research involving the properties of coordination compounds, as well as aspects of environmental chemistry. Currently, they are investigating the removal of metals and organic compounds from water by means of supported chelatings agent. 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 six grandchildren.

Sponsors

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Phone: (813) 974-2804

Graduate Talks Morning Session (CHE 100)

9:00- 9:15 AM **Douglas Franz**
Accurate, Polarizable H2 Sorption Modeling in rht-MOF NOTT-112.

9:15- 9:30 AM **Adam Hogan**
Developing Next Generation Classical Models for Ethylene and Acetylene.

9:30- 9:45 AM **Alfredo Peguero-Tejada**
Investigating Methyl Group Effect on DNA Structure via Enhanced Sampling of Base Pair Parameters.

9:45- 10:00 AM **Break**

10:00- 10:15 AM **Fiona Kearns**
An Efficient and Accurate pKa Calculator Using the QM-NBB Method.

10:15- 10:30 AM **Arthur Maknenko**
Guest interactions with a flexible host saccharide cavity via NMR.

10:30-10:45 AM **Alekhya Nimmagadda**
Synthesis of Biodegradable Polycarbonate Nanostructures with Selective Lysis against Gram Positive Bacteria.

Graduate Talks Afternoon Session (CHE 100)

3:15-3:30 PM **Ankush Kanwar**
Studies aimed at the synthesis of Anti-infective agents

3:30- 3:45 PM **Benjamin Eduful**
Synthesis of Novel Agents for the Treatment of Infectious and Neurodegenerative Diseases.

3:45- 4:00 PM **Jeanine Yacoub**
Search for Drug Targets and Possible Treatments for Toxoplasmosis.

4:00- 4:15 PM **Break**

4:15- 4:30 PM **Jennifer Borja**
New Derivatives of N-Alkythio Beta Lactams New Multimodal Functionality targets MRSA.

4:30- 4:45 PM **Linda Barbeto**
Studies Aimed at the Synthesis of Hsp90 Inhibitors as Antileishmaniasis Agents.

4:45- 5:00 PM **Seyedmorteza Hosseyni**
Gold Catalyse New Reaction Discovery.

The Barbara and Dean F. Martin Poster Session
CHE 101A

Graduate: Group GP All Disciplines

The Jianfeg Cai Poster Session
CHE 103

Undergraduate: Biophysical (BP), Chemical Education (CE), Computational (CO), Inorganic (IN), Physical (PC)

The ACS Tampa Bay Local Section Poster Session
CHE 101A

Undergraduate: Analytical (AN), Biochemistry (BC), Organic (OR), Natural Products (NP)

GRADUATE TALKS

GT-01 **Douglas Franz**[1], Katherine A. Forrest[1], Tony Pham[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Accurate, Polarizable H2 Sorption Modeling in rht-MOF NOTT-112

Isothermal grand canonical Monte Carlo (GCMC, (μVT)) simulations of H 2 sorption were performed in the NOTT-112, an rht-metal–organic framework (MOF) that consists of Cu 2+ ions coordinated to 1,3,5-tris(3,5-dicarboxy[1,1-biphenyl]-4-yl)benzene ligands. Three different H2 potentials of increasing complexity were used for the simulations to elucidate the sorption mechanism in NOTT-112. Reasonable agreement with the experimental H2 sorption isotherms, isosteric heat of adsorption (Qst), and H2 –Cu2+ interaction distances were obtained for only the model that includes explicit many-body polarization. Although most traditional MOF–sorbate simulations include only repulsion/dispersion and permanent electrostatic energetics, it is shown herein that polarization is required for more accurate simulated H2 uptakes, Qst values and proper determination of the H2 sorption mechanism in NOTT-112.

GT-02 **Adam Hogan**[1], Tony Pham[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Developing Next Generation Classical Models for Ethylene and Acetylene

Accurate and transferable classical models for ethylene and acetylene have been developed from first principles with emphasis on applications in separations. Three different models for each molecule were developed with varying levels of sophistication, allowing for comparative studies and backwards compatibility with existing force fields. The resulting models are then shown to accurately reproduce various experimental data, including both homogeneous and heterogeneous environments.

GT-03 **Alfredo Peguero-Tejada**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Investigating methyl group effect on DNA structure via enhanced sampling of base pair parameters

We are developing an efficient method for the calculations of DNA base pair parameters in molecular dynamic simulations. These six parameters (shear, stretch, stagger, buckle, propeller, and opening) describe the relative geometric orientation of the DNA bases. The method does not use idealized base pairs and uses a reduced representation of DNA, which results in faster calculation of the needed derivatives. Use of the method, which achieves excellent correlation with 3DNA, is illustrated by umbrella sampling the propeller parameter on the middle step of DNA dodecamers. The Dickerson dodecamer and related sequences with and without uracil replacements were simulated to analyze possible thymine-methyl group steric influences on the propeller angle.

GT-04 **Fiona L. Kearns**[1], Phillip S. Hudson[1], Stefan Boresch[2], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Computational Chemical Biology, University of Vienna

An Efficient and Accurate pKa Calculator Using the QM-NBB Method

A protein's function is tightly linked to acid/base residues that play critical roles in both ligand binding and catalysis. The relative stability of protonated/deprotonated forms is highly sensitive to changes in electrostatics and conformation. Modeling deprotonation via free energy simulations (FES) is therefore challenging due to the need to accurately represent inter- and intramolecular interactions, often requiring quantum mechanics, while adequately sampling conforma- tional space, often requiring long simulations. Not surprisingly, FES methods are not robust enough to reliably and routinely predict pKas. We have devised a pKa calculation protocol utilizing the quantum mechanical non-Boltzmann Bennett's Acceptance Ratio (QM-NBB) method and we have applied this protocol to investigate pKas of typically challenging catalytic residues in enzymes. We have repeated this calculation employing MM simulations reweighted to SCC-DFTB. Results were in agreement with those from past work (pKa = 7.8 ± 0.1) while also providing a 60% reduction in computational expense.

GT-05 **Arthur Maknenko**[1], Ali A. Husain[1], Kirpal S. Bisht[1]
[1]Department of Chemistry, University of South Florida

Guest interactions with a flexible host saccharide cavity via NMR

Solution state NMR determines ligand/protein (guest/host) interactions via changes in chemical shifts, relaxation of the free/bound partners, water mediated magnetization transfer and molecular diffusion. Simpler moieties, like small organic molecules and cyclodextrins also undergo guest/host interactions and are monitored via 1H and Diffusion Ordered Spectroscopy (DOSY) NMR. Our synthetic host, Resorcin[4]arene Cavitand Glycoconjugate (RCG) behaves similarly to β-CD, based on complex equilibrium, Kc, and association, Ka, constants. Thermodynamic values, ΔG°, ΔH° and ΔS° indicate that guest interaction occurs in the top saccharide pseudo-cavity of the host.

GT-06 **Alekhya Nimmagadda**[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Biodegradable Polycarbonate Nanostructures with Selective Lysis against Gram Positive Bacteria

The resistance developed by the bacteria against antibiotics has become in a major concern in Health care department. Therefore there has been a significant interest in the development of antimicrobial cationic polymers due the ease of manufacture and low manufacture cost compared to small antimicrobial peptides (AMPs). Herein I present the synthesis of amphiphilic polycarbonate nano structures which had a potent antimicrobial activity against gram –positive bacteria. Fluorescence and TEM studies suggest that these polymers are likely to kill bacteria by disrupting bacterial membranes and they are highly selective which was confirmed from the hemolytic studies.

GT-07 **Ankush Kanwar**[1], Nicholas Wallace[1], Dr. James Leahy[1], Dr. Dennis Kyle[2], Brian Vesely[2], Tommy Mcgaha[2]
[1]Department of Chemistry, USF
[2]Department of Global Health, USF

Studies aimed at the synthesis of Anti-infective agents

The need for new anti-infective drugs is greater than ever before owing largely to the emergence of multidrug resistance in common pathogens as well as the rapid emergence of new infections. Leishmaniasis and malaria are two of the most common infectious diseases which affect large populations, especially in less developed countries. Leishmaniasis is a parasitic disease caused by the protozoan parasite Leishmania donovani and transmitted through the bite of sandflies. Hsp90, a chaperone protein, is critically important for the growth of protozoan parasites in their hosts and differs from their mammalian counterparts. Based on a high throughput screen, we identified a known human Hsp 90 inhibitor that showed antileshmanial activity. We have prepared a series of analogs to explore and improve the activity and selectivity of this series. Plasmodium is the parasitic protozoa that cause malaria. It also involves two hosts (mosquito and mammals) during its life cycle. Gametocytes (mature sexual stage) are present in the blood of infected vertebrate hosts while gametogenesis and formation of diploid zygotes only occurs in the gut lumen of vector mosquitoes. It has been reported that the process of gametogenesis is induced by xanthurenic acid which is present in the gut of the mosquito. Xanthurenic acid and a series of analogs have been synthesized with the aim of impeding the transmission of malaria.

GT-08 **Benjamin Eduful**[1], Catherine Costa[1], Melissa Chin[1], Dennis Kyle[2], David Khan[3], James Leahy[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Public Health, University of South Florida
[3]College of Medicine and Molecular Medicine, Byrd Institute, University of South Florida

Synthesis of Novel Agents for the Treatment of Infectious and Neurodegenerative Diseases

In spite of the great advances made by drug discovery scientists in transforming deadly human diseases into curable ones, treatments options for diseases such as Leishmaniasis and Alzheimer's are either ineffective or not available. For example, Leishmaniasis is transmitted through the bite of an infected Sandfly and has been classified as the 9th greatest disease burden among tropical diseases, with an estimated 1.3 million new cases and 25000 deaths annually. Current treatment options include Antimony, Amphotericin or Pentamidine, but none is particularly effective and are toxic. Alzheimer's is the leading cause of dementia and the most prevalent neurodegenerative disease, affecting more than 40 million people worldwide and has been classified as the 6th leading cause of death in the US. It results from the accumulations two highly toxic proteins (β-amyloid and tau) in the brain. There is currently no cure and available treatment options are symptomatic. To this end, our drug discovery efforts are towards the synthesis of novel class of agents active against; 1) Heat Shock Protein 90 (Hsp90) - shown to be the most abundant protein in the protozoan that causes Leishmaniasis – being involved in a variety of morphological process, and 2) 'Slingshot' (SSH1) - a protein proven to contribute to the formation of β-amyloid peptides in alzheimer's.

GT-09 **Jeanine Yacoub**[1], Travis Bland[1], Michael White[2], James Leahy[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Molecular Medicine & Global Health, University of South Florida

Search for Drug Targets and Possible Treatments for Toxoplasmosis

Toxoplasmosis is an opportunistic disease caused by the protozoan parasite Toxoplasma gondii. In immunocompromised patients, the parasite is dangerous and can cause symptoms such as encephalitis, cognitive disorders, seizures, and death. Combination drug therapy is the usual treatment for toxoplasmosis; however, patients suffer from problems of intolerance, allergic reactions, and cytotoxicity. In an effort to identify new drug targets for toxoplasmosis, a series of compounds have been synthesized that can be used as tools to probe the unique pathways used by T. gondii to survive in the human host. One class of these compounds is pyridinyl imidazoles, which have been shown to be active against T. gondii MAP kinases. To set up a protein pull down assay, a biotinylated linker was synthesized. We have also synthesized a compound that's being used to study the pathways involved in the most proliferative form of T. gondii.

GT-10 **Jennifer Borja**[1], Biplob Bhattacharya[1]
[1]Department of Chemistry, university of South Florida

New Derivatives of N-Alkythio Beta Lactams New Multimodal Functionality targets MRSA.

See email Methicillin Resistant Staphylococcus aureus, (MRSA) is one of the ESKAPE pathogens. MRSA infections pose a serious risk to not only the immune compromised or elderly persons causing a skin scrape can be life threatening. Over $ 9.6 billion in additional healthcare related costs was spent on MRSA related hospitalizations and over 18, 000 deaths in one year. This generation of novel derivatives of N-alkylthiolated -lactams are multimodal, anti-MRSA agents which primarily inhibits Fatty Acid- biosynthesis and are believed to exhibit broad spectrum antibacterial and antifungal bioactivity based on their substituent structures known functions.

GT-11 **Linda Barbeto**[1], James W. Leahy[1], Andrea Lemus[1], Carla O'Neal[1], Dennis Kyle[2], Tina Mutka[2]
[1]Department of Chemistry, University of South Florida
[2]Department of Global Health, University of South Florida

Studies Aimed at the Synthesis of Hsp90 Inhibitors as Antileishmaniasis Agents

Leishmaniasis is a widespread parasitic disease prevalent in less developed countries for which few effective treatments are available. Studies have shown that compounds active against Hsp90 are also active against Leishmania donovani cells. Our lab is currently investigating Hsp90 inhibitors with the goal of discovering new antileishmaniasis agents. Our project consists of making analogs to the tetrahydroindazole core of the Hsp90 inhibitor SNX 2112 in order to explore increased binding within the active site in an attempt to increase antileishmanial activity.

GT-12 **Seyedmorteza Hosseyni**[1]
[1]Department of Chemistry. University of South Florida

Gold catalyse new reaction discovery

Abstract: Gold-catalyzed reactions developed very fast during the last decade. Enyne cycloisomerization is a fundamentally important process in chemistry research due to its ability to achieve complex architectures through simple steps and its mechanisms that often reveal new chemistry insights. Implementation of enyne cycloisomerization for synthesizing complex building blocks and its mechanistic insight is advancing rapidly. Our research group establishes methods in synthesizing important building blocks in natural product by cycloisomerization of enynes. Allenes, Furanes, Spiro systems and a couple of other complicated molecules has successfully made by triazole-gold as chemoselective and stable catalyst.

GRADUATE POSTERS

GP-01 **Garrett Craft**[1]
[1]Department of chemistry, University of South Florida

Rheological analysis of food thickeners for patients with dysphagia

This rheological work investigates the interactions of sucralose, sorbitol, and polyethylene glycol with the carbohydrate matrices of food thickeners. Food thickeners are necessary to increase the apparent viscosity of foods for patients with dysphagia (a swallowing disorder) and mitigating aspiration risk. Thickening is usually obtained with the incorporation of a starch (a combination of linear amylose and branched amylopectin) or xanthum gum (a branched polysaccharide isolated from the bacterium *Xanthomonas campestris*) into the food, where physical interactions yield weak structures which resist deformation and flow from applied strain. In addition, hospitals often incorporate laxatives into their foods for patients and it has been noted that the polymeric PEG (polyethylene glycol) deviates from the behavior of its small-molecule active ingredient cousins sucralose and sorbitol in its apparent thinning of the food thickener formulations. It's of great interest to rheologicaly probe the reasons for this deviation and disruption of internal thickener structures by a polymeric species, and to suggest, perhaps, a solution for hospitals so they can provide formulations which remain efficacious and safe for patients.

GP-02 **Alekhya Nimmagadda**[1]
[1]Department of chemistry, University of South Florida

Synthesis of Biodegradable Polycarbonate Nanostructures with Selective Lysis against Gram Positive Bacteria

The resistance developed by the bacteria against antibiotics has become in a major concern in Health care department. Therefore there has been a significant interest in the development of antimicrobial cationic polymers due the ease of manufacture and low manufacture cost compared to small antimicrobial peptides (AMPs). Herein I present the synthesis of amphiphilic polycarbonate nano structures which had a potent antimicrobial activity against gram –positive bacteria. Fluorescence and TEM studies suggest that these polymers are likely to kill bacteria by disrupting bacterial membranes and they are highly selective which was confirmed from the hemolytic studies.

GP-03 **Adam Aboalroub**[1], Dimitra Keramisanou[1], Randy Larsen[1], Ioannis Gelis [1]
[1]Department of Chemistry, USF

Molecular mechanism of protein kinase sorting by Cdc37, the kinome-specific cochaperone of Hsp90

The kinome specific cochaperone,Cdc37, is involved at a late stage of kinase folding, to recruit kinases to Hsp90. Despite the striking sequence and structural homology within the kinase family, there is an intriguing substrate selectivity, where some kinases require the Hsp90-Cdc37 pair, while others not. We have used a combination of NMR and fluorescence spectroscopy, together with limited proteolysis coupled to mass spectrometry to reveal the molecular basis of the underlying selectivity. We demonstrate that within the Hsp90-Cdc37 pair, Cdc37 is able to sense the thermal stability of protein kinases.It does so, by inducing local unfolding only to bona fide substrates -that are inherently less stable- and producing ametastable conformationthathas high affinity for Hsp90. Chaperone-independent kinases -that are inherently stable- although recognized by Cdc37, do not undergo a conformational transition and readily dissociate. Thus, Cdc37 subjects kinase catalytic domains to a controlled conformational stress as a mechanism for sorting client kinases.

GP-04 **Elizabeth Yancey**[1], Renee Fleeman[2], Les N Shaw[2], Bill J Baker[1]
[1]Department of Chemistry and Center for Drug Discovery and Innovation, University of South Florida
[2]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida

Optimization of the Fungal Metabolome via Epigenetic Modification

Epigenetic manipulation of the fungal metabolome helps us to increase their production of pharmaceutically relevant molecules. There are many types modifications that can be induced, each with unique result on the epigenome, including histone modification. Ten different fungal isolates were studied in ten inhibition conditions of histone deacetylase (HDAC) to observe what control, if any, each inhibitor provided on the expression of fungal metabolites. Statistical analysis of LC/MS-QToF data was used for comparison of the inhibitors across different fungal samples, allowing for the identification of the best HDAC inhibitor for eliciting bioactive chemistry from fungi.

GP-05 **Anne-Claire Limon**[1]
[1]Department of Chemistry

Isolation of Metabolites from Epigenetically Modified Mangrove Fungi for Antiinfective Drug Discovery

The chemical survival mechanisms used by fungi offer a potential axis for research to find new drugs. Epigenetic regulation is a key mechanism to orchestrate the expression or suppression of gene activity. Manipulating these mechanisms offers new opportunities to express down-regulated secondary metabolite genes and has the potential to generate new potent and novel metabolites. Screening studies in our labs have shown that fungi from Floridian mangroves, cultured on rice in the presence of epigenetic regulators, exhibited activity against microbial agents. A DNMT treated fungus was active in ESKAPE screening. Through a bioassay-guided sequence compiling extractions, partitions, and chromatographic methods, the separation of a crude extract material has shown potential new chemistry.

GP-06 **Sylvia Soldatou**[1,2], Renee Fleman[3], Lindsey N. Shaw[3], Bill J. Baker[2,4]
[1]National University of Galway, Ireland
[2]Department of Chemistry, University of South Florida
[3]Department of Cell Biology, Microbiology,and Molecular Biology, University of South Florida
[4]Center for Drug Discovery and Innovation, University of South Florida

Anti-MRSA natural products from an epigenetic modified Florid-ian mangrove-associated fungus

The ESKAPE pathogens are responsible for the majority of nosocomial infections and are resistant to most antibacterial agents. Our lab is interested in the isolation and characterisa-tion of secondary metabolites from mangrove-associated fungi which are active against the ESKAPE pathogens. Moreover, we are interested in enhancing the bioactivity of these sec-ondary metabolites by epigenetic regulation using HDAC and DNMT inhibitors. During this project a suite of new and known compounds with anti-MRSA activity have been uncovered. The endophytic fungus was cultured under the regulation of an HDAC inhibitor on rice. The fungal culture was extracted with EtOAc and the crude extract was partitioned between water and EtOAc. The EtOAc partition showed activity against MRSA at 5 µg/ml and was subjected to MPLC giving five fractions. All bioactive MPLC fractions were purified through HPLC leading to the isolation of at least four new and know compounds, exhibiting moderate activity against MRSA.

GP-07 **Andrew J. Shilling** [1,2], Jacqueline L. von Salm[1,2], Ryan M. Young[1,2], Charles D. Amsler[3], James B. McClintock[3], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida
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Isolation and characterization of halogenated monoterpenes: investigating the relationship between Plocamium cartilagineum and Paradexamine fissicauda

Plocamium cartilagineum is a widely occurring red algal species responsible for structuring many benthic marine ecosystems found in the shallow waters of Antarctica. This rhodophyte is known to produce many cytotoxic polyhalogenated monoterpenes thought to serve as feeding deterrents to sympatric algal consumers. However one remarkable amphipod Paradexamine fissicauda, has been shown to consume P. cartilagineum; and is not only tolerating these chemical defenses, but sequestering halogenated monoterpenes for its own defense. In order to gain a greater understanding of this relationship, numerous halogenated monoterpenes were isolated from P. cartilagineum collected at Palmer Station in Antarctica for subsequent field-based feeding assays and further metabolomics studies. Monoterpenes within P. cartilagineum extracts were targeted using HPLC purification and characterized using 1D and 2D NMR as well as GC/MS analysis. During this investigation several previously reported halogenated monoterpenes were isolated while multiple new structures of the same class were also found.

GP-08 **Santana A. L. Thomas**[1], Renee Fleming[2], Lindsey Shaw[2], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida
[2]Cellular, Microbiology and Molecular Biology Department, University of South Florida

Isolation of Induced Bioactive Secondary Metabolites via Epigenetic Modification

Fungal endophytes have gained increasing interest over the past two decades as a source of new bioactive natural products. As it meets a developing source of secondary metabolites, this makes it an ideal focal point for new natural products. Small molecules such as secondary metabolites are targets for potential new drug candidates especially for antibiotic resistant disease. Enterococcus faecium, Staphylococcus aureus, Klebsiella species, Acenitobacter baumanii, Pseudomonas aeruginosa, Enterobacter species (ESKAPE) pathogens are classed as the most infectious diseases because of the lack of effective antibiotics for these pathogens. The need for new drugs can benefit from new methods such as epigenetic regulation of fungal metabolism. In this project, a sample of a black mangrove leaf stem was plated on Sabouraud dextrose agar for isolation of the fungal endophytes. Once isolated it was treated with sodium butyrate, a histone deacytalase (HDAC) inhibitor, resulting in a bioactive extract against Methicillin-Resistant Staphylococcus aureus

GP-09 **Matthew A. Knestrick**[1,3], Renee Fleeman[2], Glenda Ooroth[13], Lindsey N. Shaw[2], Bill J. Baker[1,3]
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New, antibiotic tetramic acids isolated from a epigenetically modificed marine fungal endophyte

Methycilin-resistant Staphylococcus aureus (MRSA) is a common, deadly bacterial pathogen, causing more fatalities in US hospitals than HIV/AIDS and tuberculosis combined. In the face of increasingly resistant pathogens like MRSA, there is a dire need for new and novel drug candidates. Our search for new chemodiversity focuses on coastal and marine-margine mangroves that are rich with endophytic fungi. Our endophyte collection has been cultivated with and without epigenetic regulation to elicit latent secondary metabolite pathways. A fungal strain, KML14-75MG, isolated from the mangrove Pandanus spiralis, was identified for its activity against MRSA. KML14-75MG was cultured on rice treated with a DNA-methyltransferase (DNMT) inhibitor known to upregulate secondary metabolite pathways. The extract was purified using a bioassay-guided fractionation approach. New and known compounds were isolated, including a suite of tetramic acids with potent activity against MRSA. Epigenetic regulation elicited the production of new compounds not present in the untreated fungal strain.

GP-10 **Alison H. Hughes**[1], Renee Fleeman[2], Lindsey N. Shaw[2], Bill J. Baker[1]
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[2]Department of Cell Biology, Microbiology and Molecular Biology, University of South Florida, Tampa,

End-o' MRSA: Isolation of anti-bacterial compounds from a marine endophytic fungus.

Natural products have been an inspiration for drugs for decades, with 25% of NMEs (New Molecular Entity) approved since 1930 being sourced from microbes. With anti-biotic resistance becoming ever more prevalent amongst pathogenic microbial species, the race to find new therapeutics is gaining speed. As a result, we focus on harvesting new defensive metabolites from marine endophytic fungi through epigenetic modification. A large-scale rice culture, treated with the epigenetic inhibitor, is extracted with ethyl acetate and partitioned to remove water-soluble media components. These extracts are tested against a spectrum of infectious diseases, including the ESKAPE panel. Bioassay-guided isolation of one particular fungus, treated with DNMT inhibitor, has afforded a suite of anti-bacterial compounds with moderate activity against Methicillin-resistant S. aureus (MRSA). This microbe alone is responsible for over 19,000 deaths per year and is commonly referred to as a "superbug" due to its increasing resistance to therapeutics.

GP-11 **Zachary Shultz**[1,2], Grant Lawrence[1,2], Luciano Laratelli[1,2], Vincent Roth[1,2], Dr. James Leahy[1,2]
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The Claisen Rearrangement as a Template for Natural Product Synthesis

Nature produces structurally diverse and complex molecules with a wide variety of applications that attract the synthetic community. In order to exploit these applications and further study the natural products, they need to be accessible by means other than nature. Tremendous synthetic efforts and new methodology over the last two centuries have provided novel approaches to the molecules nature provides. Amongst these efforts was the discovery of the Claisen rearrangement by Rainer Claisen in 1912. This [3,3]-sigmatropic rearrangement of allyl vinyl ethers with stereocontrol is a powerful carbon-carbon bond forming reaction that has been applied to a vast number of total syntheses and has maintained its utility over the course of time. Modifications and advances to the Claisen rearrangement have extended its scope to many enantioselective natural product total syntheses. Our efforts towards the synthesis of the membranolides and members of the cannabinoid family utilizing Claisen rearrangements will be highlighted.

GP-12 **Andrea Lemus**[1], Ronald Swonger[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Pentamidine Analogs as Potential Leishmaniasis Treatments

Leishmaniasis is a parasitic disease caused by protozoa of the genus Leishmania. The disease is transmitted by the bite of an infected female sandfly. Leishmaniasis is considered a neglected tropical disease with two million new cases every year. It is prevalent in less developed countries where there are limited effective treatments available. There are three main types of leishmaniasis, and visceral leishmaniasis is considered the deadliest. Current treatments for leishmaniasis include pentavalent antimony compounds and Amphotericin B, but these are often toxic and expensive. Pentamidine is another drug used, but it also exhibits toxicity problems. In an effort to create new compounds to combat leishmaniasis, we have worked on synthesizing compounds using pentamidine as a scaffold for new analogs. Pentamidine has a simple structure and has great potential for optimization. We expect that the compounds made in this lab can show improved activity and other pharmacokinetic properties compared to pentamidine.

GP-13 **Boliang Dong**[1], Yumeng Xi[2], Yijin Su[2], Novruz G Akhmedov[2], Jeffrey L. Petersen[2], Xiaodong Shi[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Chemistry, West Virginia University

Vinyl-Cyclopropane Ring Opening as Facile process for the Synthesis of Substituted Cyclopentenes

Vinylcyclopropane represents a class of cyclopropane derivatives that possesses high synthetic value. An efficient synthesis of substituted cyclopentenes through gold/gallium-catalyzed annulation of 1,3-dicarbonyl compounds and cyclopropylacetylenes is achieved. This tandem reaction consists of a gold-catalyzed Nakamura reaction, a catalytic dienol-enone tautomerization, and a gallium-catalyzed vinylcyclopropane (VCP) rearrangement.

GP-14 **Sri Krishna Nimmagadda**[1]
[1]Department of Chemistry, University of South Florida

Desymmetrization of 4-substituted Cyclohexanones to Novel Axially Chiral Cyclohexylidene Oximes

First enantioselective synthesis of novel axially chiral cyclohexylidene oximes has been achieved by the reaction of 4-substituted cyclohexanones with aryloxy amines catalyzed by chiral BINOL strontium phosphate complex with excellent yields and high enantioselectivities.

GP-15 **Yassin Elbatrawi**[1], Juan Del Valle[1]
[1]Department of Chemistry, University of South Florida

"Electrophilic amination route to chiral hydrazino acids and macrocyclic N-amino peptides"

"Hydrazino acids offer the advantage of adding amino groups to any native peptide sequence. These additional amino groups could be deployed in a range of different strategies to achieve structural rigidification of the native peptide into beta-sheet like secondary structures. Hydrazino acids could be prepared via different routes with the most direct route being via electrophilic amination where any amino acid can be reacted with a source of electrophilic nitrogen bearing the desired protecting group (e.g Boc, Moc, Alloc,…etc) . Our research encompasses the use of an N-Boc protected oxaziridine reagent as the source of electrophilic nitrogen to prepare the corresponding N-Boc protected hydrazino acids which were then incorporated in a model dihydrazinopeptide. Crystal structure of the peptide interestingly showed a dimer with dihedral angles resembling an anti-parallel beta-sheet secondary structure. We are currently exploring the effect of macrocyclic tethering on the dihydrazinopeptide for further implementation into medicinally relevant peptides".

GP-16 **Ali Husain**[1], Kirpal Bisht[1]
[1]Department of Chemistry, University of South Florida

Molecular Cage arcerands using tandem Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC) reaction

The rigid form structure of resorcin[4]arenes "cavitands" provide an ideal structural platform for attaching and directing B-D-glucopyranoside moieties. The spatial directionality of the B-D-glucopyranosideoffered by the cavitand core delivered so-called a pseudo-cavity that have the ability to act as molecular vessel to accomadate water-insoluble hydrophobic species in aqueous environment. The utility of these glycocavitands were demonstrated as

GP-17 **Arthur Maknenko**[1], Ali A. Husain[1], Kirpal S. Bisht[1]
[1]Department of Chemistry, University of South Florida

Guest interactions with a host saccharide cavity via NMR

X-ray crystallography provides a molecular snapshot of a well defined compound or system with atomic level resolution, however, crystallization is often problematic and time consuming. Solution state Nuclear Magnetic Resonance (NMR) is a convenient alternative, because it only requires the molecule of interest to be soluble in a variety of commercially available solvents. In solution, simple organic compounds and macromolecules undergo guest/host interactions which are monitored via 1H and Diffusion Ordered Spectroscopy (DOSY) NMR. We compared the interaction between a common guest, vanillin, a naturally occurring host, β-cyclodextrin (β-CD) and a synthetic one, Resorcin[4]arene Cavitand Glycoconjugate (RCG). Based on complex equilibrium, Kc, and association, Ka, constants, β-CD and RCG form similar vanillin complexes. The thermodynamic values, ΔG°, ΔH° and ΔS° indicate that guest interaction occurs in the saccharide portion of either host.

GP-18 **Seyedmorteza Hosseyni** [1]
[1]Department of Chemistry. University of South Florida

Gold catalyse Allene and furan synthesis

Abstract: In the last decade, there has been a rapid growth of interest in homogeneous gold catalysis. Triggered by the breakthrough example of ambient alkyne hydration (Teles hydration), the predominant reactivity of gold catalysts was identified to be a highly effective p-acid toward alkyne, alkene and allene activation. In general, compared to intramolecular functional group rearrangements, transformations that enable reactions between multiple components (intermolecular) is of greater interest because it allows a rapid increase of structural complexity through the accumulation of functionalities. However, like other catalytic systems, gold catalysis has encountered unbalanced development between the intramolecular transformations (far more advanced) and their intermolecular counterparts (much less developed). Herein, we report the successful intermolecular propargyl alcohol addition to alkyne using the triazole–gold.

GP-19 **Matthew Sarnowski**[1], Yassin Elbatrawi[1], Juan Del Valle[1]
[1]Department of Chemistry, University of South Florida

Synthesis and Conformational Analysis of N-Amino Peptides (NAPs)

Recently, we designed a new class of chiral α-hydrazino acids that can be chemoselectively incorporated into a growing peptide chain on solid support. We reasoned that the propensity of these functional groups to participate in hydrogen bonding could be exploited to enforce intramolecular interactions that yield stabilized extended structures. Here, we describe the synthesis and conformational analysis of β-hairpin model peptides featuring backbone N-amination. NMR, CD, and X-ray crystallographic data will be presented. Unique sheet-like structures held together via intermolecular hydrogen bonds were observed in the X-ray crystal structure of a NAP dimer, which to our knowledge represents the first structure of this type reported for N-substituted peptides. These results suggest that NAP linkages can be utilized to control both local backbone geometries and longer-range intermolecular interactions, and also represent a new chemical handle for peptide chemical diversity.

GP-20 **Ying He**[1], Xiaohan Ye[1], Yanwei Zhang, Xiaodong Shi[1]
[1]Department of Chemistry, USF

1,2,3-Triazole amine as directing group in promoting catalytic oxidative C–H olefination under aerobic conditions

Transition metal catalyzed C-H activation has been widely applied as an efficient approach in complex molecule synthesis. In this work, a practical ortho C–H olefination of phenyl acetic acid derivatives was achieved with a 1,2,3-triazole auxiliary directing group. Good to excellent yields were achieved with O2 as terminal oxidant. Other bidentate directing groups, such as 8-aminoquinoline, gave poor reactivity under this aerobic condition, highlighting the unique reactivity of triazole in promoting C–H activation.

GP-21 **Abiola Jimoh**[1], Xiaohan Ye[1], Lukasz Wojtas[1], Xiaodong Shi[1]
[1]Department of Chemistry, University of South Florida

Highly Efficient Triazole-Based Hoveyda-Grubbs Type Complexes for Olefin Metathesis

Olefin metathesis is no doubt one of the most successful organic transformations since the past few decades for the formation of C=C bonds. A series of highly notable catalysts have been deeloped ranging from the Mo-based Schlock catalyst to Ru-based Grubbs (I and II) catalysts as well as the Ru-based Hoveyda-Grubbs (I and II) catalysts. Despite the great modifications and progress in the metathesis catalysis, challenges of catalysts stability, lower reactivity of very stable catalysts and E/Z selectivity seem elusive. Rationally designed triazole-based Ru catalysts are reported for efficient olefin metathesis reactions. The new complexes contain carbene-triazole chelating ligands and can be synthesized in one step from commercially available precursors in 85-95% yield. X-ray shows the triazole-carbene ligand forms a five-membered ruthenocycle which enables the formation of four-membered metathesis transition. The catalysts were applied to ring-opening metathesis polymerization (ROMP) and complete conversion was observed at room temperature with 0.01-0.1% catalyst.

GP-22 **Dan Utic**[1], Lindsey Shaw[2], Dan Utic[1], Renee Fleeman[2], Edward Turos[1]
[1]Department of Chemistry University of South Florida
[2]Department of Cell and Molecular Biology University of South Florida

Screening of N-Thiolated Beta-Lactams, Ciprofloxacin Analogs, and Rifamycin Analogs for Activity against Drug-Resistant Bacteria

Approximately 1600 synthetic antibacterial agents were screened for activity against the ESKAPE pathogens: Enterococcus faecium; Staphylococcus aureus; Klebsiella pneumonia; Acinetobacter baumannii; Pseudomonas aeruginosa; and Enterobacter cloacae. Our antimicrobials include N-thiolated beta-lactams, ciprofloxacin analogs, and rifamycin analogs. Results reconfirm the activity of our compounds against methicillin-resistant Staphylococcus aureus and indicate promising activity towards gram negative bacteria.

GP-23 **Alejandro Rivera**[1], **Garrett Craft**[1]
[1]University of South Florida

Synthesis and Properties of Novel Melt Processable Aliphatic Polyimides

A series of polypropylene oxide diamines (Jeffamines) were used to synthesized flexible polyimides. The aliphatic monomer introduces the flexibility required for the polyimides to have lower thermal properties that allow to be melt-processable polyimides. The polyimides were prepared by a two step polycondensation procedure from pyromellitic dianhydride (PMDA), Jeffamine D series (D230, D400, D2000 and D4000) and 4,4'-Methylenebis(2,6-dimethylaniline) (TMMDA). The lower range of Tg from 40ºC to 120ºC is below their decomposition temperature and allows the melt rheology study of high performance flexible polyimides.

GP-24 **Ali Ozcan**[1,2], Parthiban Rajasekaran[2], Rajneesh Prajapati[2], Swadeshmukul Santra[1,2,3,4]
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[2]NanoScience Technology Center
[3]Department of Material Science and Engineering
[4]Burnett School of Biomedical Sciences

Synthesis Of ZnO Nanoparticles With Non-Toxic Chelating Agents For Enhanced Biocidal Activity

ZnO Nanoparticles (NPs) are known to have antimicrobial properties against both gram positive and gram negative bacteria and it is already in use in biomedical and agricultural applications. The efficacy is affected by particle size, shape, surface charge and surface defects (i.e., higher the surface defects, higher the antimicrobial efficacy). Different ZnO NPs were synthesized using sol-gel method with non-toxic capping agents (chelates). NPs were characterized using UV-VIS, Photoluminescence (PL), FT-IR, DLS, and Zeta Potential measurements and enhanced surface defects were observed through PL measurement. High antimicrobial efficacy was observed against both gram positive and gram negative bacteria, and it is compared to metallic Zinc and bulk ZnO. Phytotoxicity studies are followed to investigate biocidal applications and no toxicity is observed at the application rate.

GP-25 **Tyler Maxwell**[1,2], Tahmina Banu[2,3], Edward Price[1,2], Jeremy Tharkur[2], Andre Gesquiere[1,2,4], Swadeshmukul Santra[1,2,3]
[1]Department of Chemistry, University of Central Florida
[2]NanoScience Technology Center
[3]Department of Material Science and Engieering
[4]CREOL, The College of Optics and Photonics

Non-cytotoxic Quantum Dot-Chitosan Nanogel Biosensing Probe for Potential Cancer Targeting Agent

Quantum dots (Qdot) biosensors have the ability to provided valuable information to researchers and also deliver cargo inside cells. In this study, we report the design and synthesis of a non-cytotoxic Qdot-chitosan nanogel composite using straight-forward cyanogen bromide (CNBr) cross-linking. The probe was characterized by spectroscopy (UV-Vis, fluorescence), microscopy (fluorescence, SEM, TEM) and DLS. This activatable ("OFF"/"ON") probe contains a core/shell Qdot (CdS:Mn/ZnS), where dopamine is bound to the surface which acts as a model drug and fluorescence quencher. Dopamine capped "OFF" Qdots can react with intercellular glutathione which releases the dopamine and turns the Qdots "ON" restoring photoluminescence. The Qdot-dopamine conjugate was coated with chitosan (natural biocompatible polymer) bound with fluorescein isothiocyanate (fluorescent dye) and folic acid (targeting). To assess cancer cell targeting, the uptake of the probe was measured on different cell lines. The probe's cytotoxicity was also evaluated on these cells and was shown to be nontoxic.

UNDERGRADUATE POSTERS

AN-01 **Angelica Clemons**[1]
[1]Department of Chemistry, University of South Florida

Analysis of pesticide compounds in surface water using LC/MS

The main objective of this research project is to analyze surface water for pesticide compounds by using Liquid Chromatography/Mass Spectrometry (LC/MS) techniques. Samples of pond water are taken from areas populated with citrus groves where active pesticide application is occurring. Samples were extracted using a liquid-liquid extraction method with dichloromethane as the solvent and analyzed in a 1:1 mixture of MeOH and H20 using LC/MS. Results have identified two pesticide compounds present in the water samples. Two prominent [M+H] peaks were detected at 279.1 and 298.1 corresponding to molecular weights of 278 g/mol and 297 g/mol. The compounds have been identified to be that of Fenthion, an insecticide with molecular weight of 278.1 g/mol, and Spiroxamine, a fungicide with molecular weight of 297.1 g/mol. The concentration of Fenthion is determined through the construction of a standard curve then calculated concentrations are compared with acceptable values

AN-02 **Kelvin Acosta**[1], Chris McKeithan [1], Dean F. Martin[1]
[1]Department of Chemistry, University of South Florida

Removal of an Antibiotic Amoxicillin from Different Aqueous Systems using Octolig®

The demand for pharmaceuticals has increased along with the rapidly increasing human population. In 2000, some 16,200 tons of antibiotics were produced in the United States, of which some 70% was used for livestock. Amoxicillin, used to manage bacterial infection is among the top five popular pharmaceuticals in the U.S. As a result, biological resistance in excess amounts may become available in waste water samples. Previous work have demonstrated that solutions of Amoxicillin in deionized water could be removed quantitatively by passage over Octolig® a polythylenediimine covalently attached to high-surface-area silica gel. Our research was concerned with testing the potential removal of Amoxicillin in various water solutions. Standard solutions were passed over chromatography columns at a rate of 10 mL per minute and 50 mL fractions were collected and analyzed for total dissolved solids and pH as well as concentration spectrophotometrically using a Shimadzu UV-2401 PV UV-Vis recording spectrophotometer.

AN-03 **Shannon Kelly**[1]
[1]Department of Chemistry, University of South Florida

Developing an in vitro Release Model for Dexamethasone-Encapsulated PLGA Nanoparticles

Current treatments for ocular inflammation require frequent intravitreal injections. This can cause increased intraocular pressure, cataracts, and endophthalmitis. Nanoparticles have reportedly shown a sustained release of drug for up to 100 days, greatly reducing the needed frequency of injection. In this study, dexamethasone nanoparticles will be prepared via nanoprecipitation and characterized. An important part of characterizing a nanoparticle formulation is conducting an in vitro release to show the sustained release of drug from the nanoparticles compared to drug solution. This is usually completed by suspending a sample of the nanoparticles in Phosphate Buffered Saline (PBS). However, in previous studies, dexamethasone has shown poor solubility in PBS, resulting in unusable data. The surfactant Tween-80 has been reported to increase the solubility of drugs in PBS. Thus, the effect of tween-80 on the in vitro release of dexamethasone nanoparticles will be analyzed.

AN-04 **Enrique Rodriguez**[1]
[1]Department of Chemistry, NMR, University of South Florida

Monitoring the Self-Aggregation of Sunset-Yellow Through the use of Chemical Shifts and Measured T1 Relaxation Times

Sunset yellow is an anionic organic dye which is able to undergo self-assembly while in an aqueous solution, this can often result in the formation of lyotropic chromonic liquid crystals (LCLCs). Although commonly known for being used in visual displays such as LCD's these crystals have important applications in various other fields. For example in recent years LCLCs have been used to enhance biological sensing of ligand-receptor binding. Aggregation has been found to be a major driving force in the production of these LCLC's thus is an important area of research. In this study the self-aggregation of sunset yellow will be monitored through the use nuclear magnetic resonance, by measuring the changes in chemical shifts and T1 relaxation times as a function of concentration.

AN-05 **Maria Parodi**[1]
[1]Department of Chemistry, University of South Florida

Study on Azo-Dye- Sunset Yellow

Sunset yellow is a mono azo organic dye able to undergo aggregation at high concentrations to form a lytotropic liquid crystal with distinct polymorphic forms based on temperature and concentration. Aggregation has been found to play a critical role in small organic molecules that can act as markers, anti tumor drugs, proteins and drug delivery and discovery thus is an important area of research. This study focuses on the effects of aggregation of sunset yellow through the use of proton nuclear magnetic resonance (1H NMR) to identify the self-diffusion coefficients though T1 Relaxation and Diffusion Ordered Spectroscopy (DOSY) at varying concentrations of sunset yellow.

AN-06 **Zachary Thomas**[1]
[1]Department of Chemistry, University of South Florida

Analyzing the Separation of two different species in DMS using SIMION

Ion-mobility spectrometry (IMS) is an analytical technique used to separate and identify atomic ions in the gas phase, based on their mobility through a carrier gas. The related technique of Differential Mobility Spectrometry (DMS) uses a varying field strength and varying time parameter to separate ions with a particular mobility dependence. A particular differential ion mobility parameter, alpha is derived from proven IMS data for Uranium and Cesium ions in a Helium carrier gas. The alpha parameters were used in SIMION 8.1, an ion optics simulation program, in DMS simulations. A method of determining alpha parameters from IMS data was further investigated. The analysis interprets the connection that IMS has to DMS through the alpha parameter.The method provides a means to determine theoretical DMS data which can be further analyzed through experimental means.

AN-07 **Ashley Windom**[1], Michelle Miranda[1], Kenyon Evans-Nguyen[1]
[1]Department of Chemistry, The University of Tampa

Characterization of a Microwave Plasma Torch With Mass Spectrometry

Ambient ionization sources developed for mass spectrometry have dramatically simplified molecular analysis. However, elemental analysis with mass spectrometry still primarily relies on complex ionization methods such as ICP. Microwave Plasma Torch (MPT) ionization has the potential to combine both molecular and elemental ionization. The current studies build on previous research using the MPT for molecular ionization, focusing on using it for elemental analysis. Elemental analysis using the MPT coupled to an ion trap mass spectrometer was characterized by building a controlled aerosol generating system. Aerosols of dissolved metals were introduced into the MPT. The influence of different parameters, such as gas flow rates, gas composition, and solution flow rates, on MPT ionization were tested using this system. These parameters changed what elements were seen and their relative intensities. The goal of these characterization studies is to move towards a fieldable MPT mass spectrometer.

BC-01 **Kevin Stutler**[1], Ryan Anderson[1], David Merkler[1]
[1]Department of Chemistry, University of South Florida

Determination of the Presence and Activity of Aralkylamine N-acetyltransferase in Tribolium castaneum

The pathway to produce palmitoyl serotonin, a fatty-acid amide in Tribolium castaneum, is catalyzed by arylalkylamine N-acetyltransferase (AANAT). In order to determine the incidence and bioactivity of this enzyme, the product of the catalyzed pathway was extracted from Tribolium by gradient chromatographic elution. It was analyzed by LC/QToF-MS to ascertain its presence in the sample. Once done, transcriptional studies through RNA extraction and RT-PCR amplification commenced on the four isoforms of Tribolium AANAT utilizing specially constructed primers that correspond to each coding sequence. After the resulting DNA was cloned and amplified, the samples were analyzed by gel electrophoresis and sequenced. This extracted DNA sequence was compared to the Tribolium genome using BLAST algorithms and, between them, a common sequence was found that was greater than 250 base pairs. This indicated that AANAT is coded for by the Tribolium genome and that it is biologically active in the organism.

BC-02 **Thuong Nguyen**[1], **Samuel McKee**[1]
[1]Department of Chemistry, University of South Florida

Reactivity of Metal Complexes with 3,5-di-Tert-Butylcatechol in the presence of Hydrogen Peroxide

Copper is an essential chemical to all living organisms. Many biological enzymes contain Cu in their active sites, such as cytochrome c oxidase. Copper can act as a redox center, going through redox cycles between Cu+1 and Cu+2. 1,10-Phenanthroline is a versatile ligand that can coordinate with various metals to produce metal complexes with different peculiar properties. 3,5-Di-tert-butylcatechol (DTBC) was used as substrate to monitor the catalytic ability of the complexes, and its oxidized product (DTBQ) formed at 410nm. When 1,10 Phenanthroline is introduced to Cu, it changes the redox potentials, showing very different activities with the presence and absence of peroxide. During presence of peroxide, 1,10-Phenanthroline acts as an activator, increases the catalytic rate. During absence of peroxide, 1,10-Phenanthroline acts as an inhibitor, reducing the catalytic rate. This simple Cu-1,10-Phenanthroline system can be used as model to investigate how different antioxidants influence the peroxidations and oxidations activities.

BP-01 **Dylan Grassie**[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

Structural Characterization of the Heme Protein Cytochrome c Mineralized within the ZIF-8 Metal Organic Framework

The ability to encapsulate bioactive molecules and enzymes within porous solid state materials has long been of interest in the development of hybrid materials for industrial applications. Metal organic materials (MOMs) are of particular interest for encapsulation of biomolecules because of their tunable dimensions, ease of synthesis and functionalizable interiors. Cytochrome c (Cyt.C) is an important target protein for encapsulation due to the stability of the protein, the relatively small size (~12 KDa) and the covalent attachment of the heme to the protein. Recently, the ability to mineralize various proteins including Cyt.C into zeolitic imidazole frameworks (ZIFs) has been reported in which the MOM forms protein encapsulated cavities. UV/Vis and steady state fluorescence measurements were obtained for the Cyt.C ZIF-8 composite to determine the impact of mineralization on the protein's conformation. The results demonstrate significant unfolding of the encapsulated protein leading to perturbations of the heme active site.

BP-02 **Cayang Zhong**[1], François Villemot[1], Alfredo Peguero[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Studying the Contribution of Local Interactions to the Secondary Structure of Chameleon Sequences Using Molecular Dynamics Simulations

Molecular dynamics simulations can be used to study small systems, such as chameleon sequences. A chameleon sequence is a small peptide that can be found as an α-helix in some proteins and as a β-sheet in other proteins. The purpose of this study is to determine how the local interactions of chameleon sequences contribute to their secondary structures. To test whether these sequences have an inherent propensity to fold either in the alpha or beta state, or if folding is driven by the entire protein, differences in conformational free energies are calculated. The confinement method provides conformational free energies by transforming the system into independent harmonic oscillators. If the sequences have an inherent propensity, it is expected for the difference in free energy between the two states to be close to zero. Otherwise, free energy difference should be similar to other proteins.

CE-01 **Giselle Irio**[1], Dr. Edwin Rivera[1]
[1]Department of Chemistry; University of South Florida

Enhancement of Organic II laboratories by the introduction of hands-on NMR spectroscopy (CHM 2211L)

Undergraduate students have only been able to theoretically assess Nuclear Magnetic Resonance (NMR) spectra in the classroom until Fall 2015. With a matching-funds grant from College of Arts an Sciences and the Department of Chemistry, Organic Chemistry II laboratories were equipped with three 60 MHz NMR spectrometers for student use. Because of the upgrades provided by the grant, students are now able to practice hands-on NMR with data collection in order to analyze and confirm their own synthetic reaction products. Student will be able to appropriately assess their lab work, and develop valuable skills, such as NMR software and NMR technology, that they can use in the scientific field. NMR is one of the most widely used characterization tools in Science. Extending these resources to the undergraduate curriculum will better prepare them for the job market, and enhance their success in future STEM endeavors. In addition, the NMR spectra from the students have helped us enhance the curriculum by evaluating reoccurring discrepancies among lab groups.

CE-02 **Kristen Eversole**[1]
[1]Department of Chemistry, University of South Florida

Attitudes, Beliefs, and Experiences of Peer Leaders in General Chemistry Peer-Led

Although the research on Peer Led Team Learning has been extensive, one area that is under-studied is the peer leaders themselves. Peer Leaders are students with a strong chemistry background that are selected to work with current chemistry students to actively engage them in the material and strengthen their understanding. Little research has been done on how peer leaders' beliefs and attitudes toward education effects their experiences and teaching behaviors over the course of the semester. In this study, the beliefs, attitudes, and motivations of the peer leaders were explored using a Teaching Belief Survey and an Internally created survey. Observations of peer leaders were then used to elucidate how these factors effected their experience through the semester. The results of this study will be used to help those running peer leading improve the program for both the leaders and the students.

CE-03 **Andrea Mapugay**[1], **Razanne Oueini**[1], Scott E. Lewis[1]
[1]Department of Chemistry, University of South Florida

The Impact of a Flipped Teaching Approach on Student Success in General Chemistry

The purpose of this project was to investigate the different teaching approaches that occur in a chemistry classroom. Throughout the semester, General Chemistry was presented with either a “flipped” or “non-flipped” teaching approach. The “non-flipped” teaching approach is a traditional model of teaching where the instructor presents content primarily through lectures. “Flipped” teaching is an approach to learning where the instructor presents content outside of the classroom by providing online resources and reading. In so doing, class time may be used to engage students in activities designed to help in understanding the content or going more in-depth into the material. This project presents a

hybrid flipped approach, designed for large classes, where half of the course content is presented outside of class and the other half is presented via lecture. This project investigates the impact of the teaching approach on student success.

CO-01 **Sean Carter**[1]
[1]Department of Chemistry, University of South Florida

Using LAMMPS to Simulate Gasses with Applications to MOF-5

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is a robust system for simulating chemical systems down to the atomic scale using both molecular dynamics and monte carlo methods. LAMMPS was used to simulate the process of equilibration in small molecular gasses such as H2 using both available paradigms, as well as a hybrid approach (mixed monte carlo and molecular dynamics), with applications to gas sorption in MOF-5 (Metal-Organic Framework 5).

CO-02 **Zachary Dyott**[1], Matthew Mostrom[1]
[1]Department of Chemistry, University of South Florida

Simulation of Hydrogen Gas Storage Using Explicit Polarization Monte Carlo Methods

Monte Carlo simulations of hydrogen sorption in MOFs and COFs can provide valuable insights into the sorption mechanism in such materials as well as the rational design of new materials targeted for specific applications. Simulations of hydrogen sorption were performed in a MOF and COF known as rht-MOF-9 and COF-1, respectively. Highly accurate and transferable potential energy functions that were developed by the Space Group were used for the simulations. The Space Group models have been found to give superior accuracy of simulation compared to traditional methods that exclude polarizability functionalities. To accurately assess the validity of our models, we compared the simulation results obtained using this polarizable model to experimental data. We found that the Space Group model which includes explicit many-body polarization effects, closely reproduces experimental data compared to models without this interaction. This suggests experimental design paradigms distinct from those suggested by traditional modeling.

CO-03 **Caroline Simmons**[1,2], Sreya Mukherjee[1], Wayne Guida[1]
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[2]Honors College, University of South Florida

Determination of Noncovalent Inhibitors of Cruzain, the Major Cysteine Protease of Trypanosoma Cruzi

Chagas disease, caused by the parasite Trypanosoma cruzi, is a parasitic illness with a death rate of more than 12,000 individuals annually. Determining new ways of inhibiting T. cruzi will diminish its effect on individuals living in susceptible, tropical areas. The major target of inhibition is the cysteine protease cruzain, a highly specific enzyme that is essential for the function of T. cruzi. Prominent sites of inhibition when targeting cruzain include the catalytic triad active site and a highly defined S2 pocket that plays a role in ligand specificity. Current studies involve the optimization of covalently binding ligands to the active site. However, by taking into account the specificity pockets and catalytic triad, computational techniques will be used to virtually screen noncovalently binding ligands. Schrodinger Suite will be used as the program to aid in optimizing these potential compounds from the National Cancer Institute Diversity Ligand set 2.

CO-04 Phillip Hudson[1], **Benjamin Pollard**[1], Michael Kemp[1], Michael Crowley[2], Henry Woodcock[1]
[1]Department of Chemistry, University of South Florida
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The role of free energy in effectively computing carbohydrate NMR chemical shifts

Computing accurate NMR chemical shifts for carbohydrates has been challenging since it requires satisfying three criteria; computing the NMR shifts with an adequate level of theory, accounting for the relevant regions of conformational space, and incorporating environmental effects. QM/MM methods were used to account for environmental effects and Boltzmann weighting to account for relevant conformations. Using β-D-Glucose, QM/MM NMR shifts at various functional and basis set pairings were computed. The main conformations of β-D-Glucose in explicit solvent were generated via CHARMM36 carbohydrate force field (C36Carb) and SCC-DFTB with 3ob parameters. Chemical shifts produced using ωB97x-D/cc-pVDZ//C36Carb gave the best overall results (1H RMSD = 0.169 ppm, 13C RMSD = 2.31 ppm). Free energy surfaces of umbrella sampled β-D-Glucose were generated with vFEP at C36Carb, SCC-DFTB/3ob, SCC-DFTB/mio, AM1, PM3, MNDO, and MNDD, and then compared to experimental with attention to conformational agreement between levels of theory.

CO-05 **Ryan Kirchoffer**[1]
[1]Department of Chemistry, University of South Florida

Allosteric Effects on the Active Site of RPE65

Stargardt's Disease is a form of juvenile macular degeneration that is caused from 11-cis-retinal and A2E buildup in the eye that has been linked to the RPE65 protein. Competitive and uncompetitive inhibition of the protein stops conversion of trans-retinyl fatty acids (TRFA) to 11-cis-retinal and has been shown to slow the progression of Stargardt's Disease. This complete inhibition also leads to night blindness due to the eye's inability to adapt to darkness. By allosterically inhibiting RPE65, 11-cis-retinal and A2E will be lowered to manageable levels,

slowing the progression of Stargardt's, and the eye's night vision is maintained. Computational chemistry was used to perform the allosteric inhibition that found an allosteric site, docked the molecule by ChemBridge ID#5624413, and ran MD on the protein-ligand complex. Before allosteric inhibition, TRFA and RPE65 had a ΔG of -7.47kJ/mol the value being lower than this after the protein's new conformation indicates success.

CO-06 **Ashley Parisi-Goldblatt**[1], M. Trent Kemp[1], H. Lee Woodcock[1], Yu Chen[2]
[1]Department of Chemistry, University of South Florida
[2]Department of Molecular Medicine

A Mechanistic Study of CTX-M-14: Understanding the Role of a Low Barrier Hydrogen Bond Through the Use of Crystallography and Computational Chemistry

Beta-Lactams are a class of antibiotics that treat bacterial infections. Antibiotic resistance is a huge problem that has occurred because of a mutation in bacteria that has developed over time. The enzyme beta-lactamase affords resistance to beta-lactam antibiotics through the hydrolysis of the beta-lactam's four-membered ring. The mechanism for which this occurs is not well understood, however it is hypothesized that a low barrier hydrogen bond (LBHB) may exist between aspartate 219 and aspartate 233 within the system and could stabilize the active site and facilitate the reaction. Through the use of crystallography and computational chemistry we were able to determine that a LBHB does exist between these residues and calculate the Root Mean Squared Fluctuations of the atoms near the active site. Based on this information, we determined that the LBHB does have an effect in stabilizing the active site of the system.

CO-07 **Christine Gambino**[1]
[1]Department of Chemistry, University of South Florida

Drug Repurposing for Alzheimer's Disease using Virtual Target Screening

Currently drug discovery is at the forefront of scientific research. Computer software can be utilized to mimic molecular interactions with specific targets. Virtual Target Screening (VTS), a novel approach, is being employed to investigate the interactions of a drug candidate with a pool of proteins to ascertain interactions other than its original target protein. The drug candidate is docked, scored and evaluated against each protein in the collection and then compared to the scores of similar molecules. The main focus of this project will be to ascertain protein targets and recognized drugs important in Alzheimer's disease so that the VTS system can be applicable for Alzheimer's disease research. Proteins such as butyrylcholinesterase, acetylcholinesterase and the NMDA receptors will be added to the VTS collection and evaluated with known drugs used to treat Alzheimer's. Future plans include developing VTS for web-based access by the worldwide research community.

CO-08 **Manuel Thornberryv**[1]
[1]Department of Chemistry, University of South Florida

Non-Boltzmann Bennet Simulations of Sodium and Potassium Solvation in Water

Ion solvation is an extremely important process in a wide variety of systems. Ion solvation plays a key role in the extreme selectivity of ion channel proteins in membranes. The selectivity of ion channel proteins cannot be described exclusively as a result of the size of the ion and it is thought that these selective properties may be due to the way that water ions coordinate to the ion. Better understanding of the processes involved with ion solvation can be reached by creating an accurate simulation of the ion solvation process. In order to examine a simple test case the ion solvation and free energies of Sodium and Potassium ions were be simulated. The free energies of solvation of the Sodium and Potassium ions were calculated using a variation of the Non-Boltzmann Bennet computational method and compared to real-world results and previous papers, as well as full QM/MM simulations.

CO-09 **Priyanka Mehrotra** [1]
[1]University of South Florida

Investigation of the Filarial Ecdysone Receptor as a Chemotherapeutic Target

This work employs computational chemistry methods to identify potential treatments for lymphatic filariasis (LF), a debilitating disease common in tropical regions which causes the accumulation of lymph. LF is caused by the filarial nematode that matures via ecdysis (molting). Molting is incited when 20-hydroxyecdysone binds to the ligand binding domain (LBD) of the nuclear ecdysone receptor (EcR), the main molting transcription factor. Thus, it is the aim of this work to identify compounds that can bind in the EcR-LBD thereby displacing 20-hydroxyecdysone and preventing molting, i.e. via competitive inhibition. ProBiS binding site similarity search, PubChem, Glide Extended Precision (XP) docking program, and Induced Fit docking studies were used to identify over 35 compounds with more favorable docking scores than 20-hydroxyecdysone, the most favorable being that of [3,5-dibromo-4-(4-hydroxy-3-phenethylcarbamoyl-phenoxy)-phenyl]-acetic acid. This list of > 35 compounds will soon be passed to a collaborator (Dr. Thomas Unnasch) for experimental verification of computational results.

CO-10 **Adam Taouil**[1], Phillip Hudson[1], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida

Efficient Calculation of Free Energies Through Non-Boltzmann Reweighting Scheme

Free energy simulation is a computational approach to calculating free energy differences in many systems ranging from simple solvation to complex reactions such as protein unfolding. The challenge in computing these free energies lie in two main concerns: (1) Accurate energetics; and (2) adequate sampling. Quantum Mechanical (QM) level representation of systems result in accurate description of inter and intramolecular forces which fulfill one of these concerns. However, the computational expense of performing QM simulations is extremely high. By implementing the Non-Boltzmann reweighting, we have conducted QM level free energy calculations, while sampling from a lower level of theory. In this study, free energy differences of gas phase blocked serine monopeptide are calculated from a Molecular Mechanical (MM) trajectory, and a SCC-3ob biased drude model trajectory (where the drude model serves as a "middle" level of theory). Our results show distinctions in backbone and residue representations across levels of theory.

CO-11 **Shana Bergman**[1], Timothy R. Lezon[1]
[1]University of Pittsburgh

Global Changes Induced by Local Perturbations

The HIV-1 capsid is a fullerene cone composed of approximately 1300 copies of a single capsomer protein. After entering the host cell, the capsid uncoats through a process that is still poorly understood, releasing its genome into the host cell and enabling replication. The host factor TRIM5α is known to bind to the capsid, induce premature coating and prevent replication. Here we explore the mechanism through which local binding events and point mutations affect the overall stability of the capsid. We approximate the capsid's potential using a coarse grained elastic network model and systematically perturb each residue in the capsomer, evaluating its effect on the global potential. We find that residues along the hexamer-hexamer interface have a strong influence on capsid dynamics, suggesting that this region may be crucial for stability and uncoating.

IN-01 **Anthony G. Giacalone**[1], Lukasz Wojtas[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

Encapsulation of Photoactive Ru(II)(2,2'-bipyridine)2(Y- Aminobutyric acid)2 into a Zn-Based Polyhedral Metal Organic Framework

Metal organic materials (MOMs) are a class of porous materials composed of organic ligand molecules linked through metal clusters (molecular building blocks) that have exceptional potential to serve as platforms for a wide array of applications including novel drug delivery, gas separation and storage, catalysis, biomimetic chemistry. Drug delivery applications for MOMs are of increasing interest as these materials can contain a high weight percent of biologically active compound within the large interior cavities while the relatively small pore sizes enables effective time release. Here we describe the development of a novel photodynamic therapy application of MOMs in which a Ru(II)(2,2'-bipyridine)2(BAM)2 (BAM=Bio-Active Molecule) cluster is encapsulated within the cavities of USF2. Exposure to white light results in the photoejection of the BAM and subsequent egress to solvent. The initial target BAM is γ-Aminobutyric acid with a controlled photorelease system involving Ru(II)(2,2'-bipyridine)2(acetonitrile)2. The characterization of these materials will be reported here.

IN-02 **Anneasha Duberceau**[1]
[1]Department of Chemistry, University of South Florida

Lanthanide MOF with a custom designed marcocylic ligand

Metal organic frameworks (MOFs) are built from metal containing nodes and organic linkers. One of the potential for MOFs that is particularly remarkable is the ability of selectivity for specific analytes or classes of analytes through systems such as molecular sieving (size exclusion)through the selection of suitable organic linkers or struts. Tetracarboxylate ligand, 1,4,7,10-tetraazacyclododecane- N, N', N'', N'''-tetra-p-methylbenzoic acid (tactmb), was used to build metal macrocyclic frameworks (MMCFs). MMCF-1 a two-fold interpenetrating a microporous Cadmium based MOF. Cu(II) and tactmb, MMCF-2 demonstrates high catalytic activity for the chemical fixation of carbon-dioxide into cyclic carbonates. MMCF-3 a lanthanum based Metal Macrocyclic Framework, the azamacrocyclic-based ligand coordinates in a tetradentate manner to four separate lanthanum ions through its carboxylate groups only, leaving the macrocycle site unoccupied. Continuing research is exploring possible synthesis conditions for new macrocycle-based ligands using 1, 4, 7, 10-tetraazacyclododecane and carboxylate-containing pendant arms, derived from isothalate and nicotinate.

IN-03 **Miles White**[1]
[1]Department of Chemistry at University of South Florida

Enzyme kinetic studies using thiostrepton and Cu (II) by method of UV/vis spectroscopy

Organometallic enzyme binding is a growing field that has an impact on drug discovery, bioinorganic chemistry, and materials sciences. Recently, the physical properties of many compounds which have metal binding capabilities are being studied. binding also changes the chemical reactivity of the compound, which can lead to more effective drugs. The focus of this research is on the oiligiopeptide and naturally occurring antibiotic, thiostrepton, which has shown metal binding capabilities. The binding of Cu2+ to thiostrepton creates a metal ligand complex. Many questions can be raised at what ratio Cu2+ binds to thiostrepton and spectroscopic methods will be used to investigate the binding of the metal to ligand and the complex's ability to oxidize over the pH spectrum. A pH plot was constructed to find the pKa of the Cu2+ thiostrepton complex and give insight into the the ideal pH at which Cu2+ thiostrepton oxidation chemistry is most

IN-04 **Timmy Thiounn**[1], Wenyang Gao[1], Shengqian Ma[1]
[1]Department of Chemistry, University of South Florida

Tuning gas adsorption behavior via arraying open metal sites in isostructural porous covalent porphyrin frameworks

Driven by ubiquitous biological functions of metalloporphyrins in nature, metalloporphyrin units are of increasing interest to be incorporated into various porous materials. In particular, metal-metalloporphyrin frameworks have been emerged into an advanced type of functional porous materials showing extensive applications in the fields of gas separation, biomimetic catalysis, thin films and light-harvesting. However, their main drawback of poor water/chemical stability casts a shadow on the further exploration in practical applications. In contrast, porous covalent porphyrin frameworks (PCPFs) featuring unique thermal and chemical stability, lead to be an alternative option of porous porphyrin-based materials. Here we demonstrate how to tune gas adsorption performances via arraying various open metal sites (Mn, Fe, Co, Ni, Cu) in isostructural PCPFs. This will establish an appealing approach to understanding the interactions between guest molecules and transition metal ions in porphyrin rings, which is particularly profitable to custom-design metalloporphyrin-based porous materials for task-specific applications in the future.

IN-05 **Jessica Dick**[1]
[1]Department of Chemistry, University of South Florida

Metal extraction from aqueous solution using porous organic polymers

The significance for the removal of heavy metals and other toxins is essential to the environment and future development. There are many types of removal processes, however, ion-exchange resins are the leading materials in this area. Ion-exchange resins have drawbacks including slow ion-exchange behavior, low capacity, uncontrolled swelling, and inefficient accessibility to ion-exchange sites. Porous organic polymers (POPs) offer a new model for ion-exchange materials that overcome these limitations. The advantages of using POPs have been shown through the assessment of their performances in extracting Hg(II), Au(II), MnO4-, and ReO4- (both used as models for Tc-99) from aqueous solution. Using UV-Vis Spectroscopy, the absorbance of various concentrations of metal solutions was examined using time-dependent studies and compared to the ion-exchange resins, Amberlyst-A26(Cl) and Amberlyst-26(OH).

IN-06 **Anthony G. Giacalone**[1], Dr. Lukasz Wojtas[1], Dr. Randy W. Larsen[1]
[1]Department of Chemistry, USF

Encapsulation of Photoactive Ru(II)(2,2'-bipyridine)2(Y- Aminobutyric acid)2 into a Zn-Based Polyhedral Metal Organic Framework

Metal organic materials (MOMs) are porous materials composed of organic ligand molecules linked through metal clusters that have potential to serve as platforms for a wide array of applications including novel drug delivery, catalysis, biomimetic chemistry, chemical, and biological sensing and environmental remediation to name a few. Drug delivery applications for MOMs are of increasing interest as these materials can contain a high weight percent of biologically active compound within the cavities while the relatively small pore sizes enables effective time release. Here we describe the development of a novel photodynamic therapy in which a Ru(II)(2,2'-bipyridine)2(BAM)2 (BAM = Bio-Active Molecule) cluster is encapsulated within the Zn-based polyhedral MOM, USF2. Exposure of the new materials to white light results in the photoejection of the BAM, and subsequent egress to the bulk solvent through the exterior pores. The initial target BAM is Y- Aminobutyric acid with a control photorelease system involving Ru(II)(2,2'-bipyridine)2(acetonitrile)2.

IN-07 **Jacob Markut**[1], Christie Tang[1], Nicholas Costantino[1], Li-June Ming*[1]
[1]Department of Chemistry, University of South Florida

Oxidative Reactivity of Fe(III) and the Fe(III)-Bacitracin Complex

Bacitracin, an antibacterial produced by some soil bacteria in the genus Bacillus, is used heavily as a topical antibiotic. Bacitracin is biologically active with many divalent metal ions, but possible interactions between bacitracin and Fe(III) have remained unexplored. While iron does have a divalent state, a state whose reactivity with bacitracin had been examined by other groups, the trivalent state is more abundant, particularly in soil. Iron, a key component of Fenton's reagent, is a highly potent oxidative agent with particular relevancy to the methods of this investigation. This study focused on forming a reactive Fe(III)-bacitracin complex that could utilize Fenton-like pathways. Complexation and oxidative reactivity with and without peroxide was determined using UV-vis spectrophotometry. Iron's oxidative strength increased after complexation and also with the addition of peroxide. Results indicated successful formation of a reactive Fe(III)-bacitracin complex with enzyme-like activity.

IN-08 **Manuel Thornberry**[1]
[1]Department of Chemistry, University of South Florida

Iron Redox Activity with Thiostrepton

Iron is a redox active metal of the utmost importance in the transport of oxygen throughout the human body. It participates in Fenton chemistry in which Fe(II) is oxidized to Fe(III) and in that process creating a hydroxyl radical. Thiostrepton is a large polycyclic oligopeptide utilized for its antibiotic properties. Thiostrepton is currently most popularly used as a topical antibiotic in the treatment of animals. This study seeks to examine the behavior of Fe(III) and its ability to perform Fenton chemistry when bound to Thiostrepton. This data is collected by referencing

the oxidation of Di-tert-butyl-catechol to Di-tert-butyl-quinone by the Quinone's distinct absorbance at 410 nm. Thiostrepton appears to act as an activator for the oxidative activity of Fe(III).

NP-01 **Brittany Thiessen**[1], Alex Cole[1], Elizabeth Yancey[1], Bill J Baker[1]
[1]Department of Chemistry and Center for Drug Discovery and Innovation, University of South Florida

Natural Products of Carijoa riisei

Punaglandins have demonstrated anti-inflammatory and antitumor activity. Originally collected in Hawaii, Carijoa (Telesto) riisei was recently collected in Clearwater Beach, Florida. Despite extensive variation between ecosystems, the octocoral possess similar chemistry, specifically between eicosanoid metabolites punaglandins and pregnane steroids. Punaglandins had not been found in Caribbean Telesto until CWR13. The sample of coral was extracted, partitioned and was separated in a series of 1H-NMR guided fractionation. Using 13C and 2D NMR experiments structures of various fractions were obtained.

NP-02 **Giannina Alvarez-Calderon**[1], Chris McKeithan[1], Dean Martin[1]
[1]Department of Chemistry, University of South Florida

Removal of a common nonsteroidal anti-inflammatory drug (NSAID) using Manganilig, a manganese (II) derivative of Octolig

Acetaminophen is a NSAID found in Tylenol. It is a very popular substance with 3.6 billion grams used in the US annually. This drug is commonly found in water treatment plant effluents. Accordingly, it seems prudent to devise methods for point-source pollutant removal so that the possibility of pharmaceutical-resistant bacteria could be minimized. Previous efforts to remove organic anions through the passage over Octolig (a transition-metal polyethylenediimines covalently attached to high surface area silica gel) were successful. Acetaminophen has a pKa value of 9.51 and showed a removal of 32.4%. Therefore, an attempt to remove this from solution was made using Manganilig, a manganese (II) derivative of Octolig. The hypothesis is that the functional group on the acetaminophen might coordinate with the manganese (II) anion and a counter anion such as hydroxide might be effective in forming the Bronsted base of acetaminophen and assist in the removal of this NSAID.

NP-03 **Steve Ferlita**[1], **Shane Clark**[1], **Prasanth Nemani**[1]
[1]Department of Chemistry, University of South Florida

Biochemical Importance of Antarctic Corals

Natural products are compounds that have been found to be beneficial to modern medicine. One such organism, a coral, Plumerella delicatessima from the Scotia Arc. After extraction, multiple purification steps including medium pressure liquid chromatography and high pressure liquid chromatography were used to isolate compounds. Nuclear magnetic resonance spectroscopy and mass spectrometry were then utilized to elucidate metabolites. Five novel diterpenes and one known compound, pukalide aldehyde, were isolated throughout this research. The compounds were all bioassayed and found to not be active against the ESKAPE pathogens. The compounds were all structurally similar to the neuromuscular toxin, lophotoxin, which has a profound paralyzing effect through its irreversible binding to the acetyl-choline receptors in the brain and muscles. Further purification are currently being carried out to isolate more of these novel compounds and further bioassays, specifically assays that target the brain, will be tested to compare their similarity to lophotoxin.

NP-04 **Dakota Becker-Greene**[1,2], **Christian Stanley**[1,2], Anne-Claire Limon[1,2]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery and Innovation, University of South Florida

Methods for the Extraction of Epigenetically Modified Fungi Active Against Infectious Diseases

Secondary metabolites of marine fungi have been found to be beneficial in inhibiting bacterial infectious diseases. Production of secondary metabolites is directly related to gene expression, which is why epigenetic regulation can be used to amplify the expression of down-regulated gene sequences present within the fungi. This can potentially generate new, effective and unique metabolites. In order to isolate pure compounds that are bioactive against the E.S.K.A.P.E. pathogens, a standard method of extraction, isolation, purification, and identification was designed. The fungal samples were grown on rice media and inoculated with epigenetic modifiers, then extracted by filtration, and purified using MPLC and HPLC. In addition, bioassay tests and proton NMR spectroscopy guided the research process towards isolating pure active compounds. So far, a DNMT treated fungal sample has yielded a bioactive fraction with 1 ug/mL activity against MRSA.

NP-05 **Aaron J. Puebla**[1], **Brittany A. Dudley**[1], Jacqueline L. von Salm[1], Andrew J. Shilling[1], Laurent Calcul[1], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida

Viability of the CDDI pure compound library as a diverse suite of potential hits in drug discovery

The pure compound library at the Center for Drug Discovery and Innovation contains a diverse and ever-growing collection of pure compounds. Currently the library has 197 compounds identified and compiled, many of which are unique and were provided by labs within the University of South Florida system. These compounds are available for testing and have already been submitted to a number of bioassays, including the ESKAPE pathogens, leishmaniasis, naegleriasis (the "brain-eating amoeba"), and tuberculosis. The CDDI collaborates with labs

at other universities to broaden its testing range for these compounds. The chemodiversity lab at CDDI is available to accept more pure compounds to add to the library, with efforts to increase chemical spacing in an already diverse compound set.

NP-06 **Natalie Dehaney**[1], **Thomasina Watson**[1], Tiara Da Silva[1], **Patrick Walther**[1], Andrew Shilling[1], Bill Baker[1]
[1]Center for Drug Discovery and Innovation, University of South Florida

Extracting Natural Products from Marine Invertebrates

Marine ecosystems are a source of incredible bio-diversity and contain many invertebrate species which produce biologically active secondary metabolites, known as natural products. The purpose of this investigation is to extract and explore the pharmacological properties of the natural compounds found in marine invertebrate organisms in the context of drug discovery. Over 320 marine invertebrate organisms have been chemically extracted and sent for testing of their potential biological activity against target diseases. By using both non-polar and polar extracting solvent schemes, the marine organisms undergo multiple rounds of extractions to generate crude extracts. Once obtained, the extracts are filtered and dried under nitrogen before being prepared in DMSO at a concentration of 30 mg/mL and sent to a variety of bioassays for efficacy against target diseases. To date, the extracts have been sent for testing against Naegleria fowleri, Leishmania donovani, Acanthamoeba, lymphatic filariasis, drug-resistant ESKAPE pathogens and cancer-cell bioassays.

NP-07 **Jose A. Jesurajan**[12], Matthew A. Knestrick[12], Bill J. Baker[12]
[1]Department of Chemistry
[2]Center for Drug Discovery and Innovation

"Structural elucidation of new compounds isolated from fungal endophytes found in Pandanus spiralis

Mangroves endophytic fungi live in harsh, variable conditions, and face many competitive stressors. To aid in survival and proliferation, these endophytes produce many unique secondary metabolites. These secondary metabolites are promising sources of new, bioactive compounds to combat drug-resistant pathogens like methycilin-resistant Staphyloccocus aureus (MRSA). One fungal strain, isolated from a mangrove tree Pandanus spiralis, exhibited potent activity against MRSA. It was grown in large scale rice-based cultures and extracted. Fractionation of the crude extract was performed with High-Performance Liquid Chromatography (HPLC) and was guided by Nuclear Magnetic Resonance (NMR) spectroscopy. From the crude extracts, many new and known compounds with potent activity against MRSA were isolated. Inactive fractions were investigated, resulting in the discovering of new and known sterols.

NP-08 **Kali Young**[1], Elizabeth Yancey[1], Bill Baker[1]
[1]Department of Chemistry and Center for Drug Discovery and Innovation, University of South Florida

Drug Discovery from Antarctic Marine Invertebrates

Drug Discovery from Antarctic Marine Invertebrates The Southern Ocean is teeming with life, and, compared to other parts of the world, is unique in many different aspects. The circumpolar current isolates the Antarctic continent, which isolates nutrients and creates a barrier to the surrounding ecosystems, subsequently creating an evolutionary division in the Antarctic marine species, most notably microbes, algae, and invertebrates, such as nudibranchs, tunicates, sponges, corals, bryozoans, molluscs, and echinoderms. The interactions between these species can be studied from a chemical perspective, providing valuable insight into the complex ecological networks they form. The molecules involved in these interactions have the added benefit of being bioactive against many different human ailments including cancer, microbial and viral infections, and tropical diseases. These unique, diverse molecules contribute greatly to our knowledge of our environment, as well as disease.

NP-09 **Katherine Pioszak**[1,2], **Manuel Bermudez-Perozo**[1,2], **Vanessa Turkson**[1,2], Sophia Estrada[1,2]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery and Innovation, University of South Florida

Bio-assays of Marine Invertebrates Against Harmful Pathogens

Since the pharmaceutical industry's withdrawal from the development of antibiotics, the task of developing new treatments has fallen largely to academia. Marine natural products are biologically active secondary metabolites produced by marine organisms, many of which possess pharmacologically relevant properties. During this investigation, roughly 320 different marine invertebrates were chemically extracted using both polar and nonpolar solvent systems to yield a variety of crude extracts. These extracts were dried, solvated in dimethyl sulfoxide and sent to various bioassays testing against a range of known disease-causing microorganisms, including ESKAPE, Naegleria fowleri, Acanthamoeba, Leishmania donovani, and lymphatic filariasis. These extracts have also recently started to undergo testing against cancer cell-lines in search of potential chemo-therapy treatments. In total, 630 different crude extracts have been sent for testing, with multiple hits against ESKAPE, Naegleria fowleri, and cancer cell-lines reported thus far.

NP-10 **Jacob Norman**[1,2,3], Dan Utic[2,3], Dr. Edward Turos[2]
[1] Department of Cell Biology, Microbiology and Molecular Biology, University of South Florida
[2]Department of Chemistry, University of South Florida
[3]Florida Native Plant Society

Investigation of Natural Products from Pterocaulon pycnostachyum

Pterocaulon pycnostachyum, commonly called coastal blackroot, is a member of the Asteraceae family and is endemic to Florida. Members of the Asteraceae family are known to contain biologically active compounds. Despite these records, P. pycnostachyum has yet to be formally studied in a laboratory setting. We have extracted Pterocaulon pycnostachyum root to isolate and elucidate the structure of any biologically active compounds.

OR-01 **Travis Bland**[1], Jeanine Yacoub[1], James Leahy[1]
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Synthesis of Shield1 Ligand for the Molecular Studies of Toxoplasma gondii

Toxoplasmosis is a parasitic disease caused by the protozoan Toxoplasma gondii. Symptoms are almost non-existent in healthy individuals but pose significant risk for the immunocompromised. Infection occurs most commonly from consumption of undercooked meat from an infected animal or from handling cat feces. The Destabilizing Domain (DD) is a 12-kDa tag that, when expressed on a protein of interest, undergoes rapid degradation in the cell by proteasomes. When Shield1 is introduced to the culture, it reversibly binds to the Destabilizing Domain tag and prevents degradation, allowing the tachyzoite form of T. gondii to persist. This method has been used to study a significant transcription factor, AP2IX-9, in the development of the bradyzoite form. AP2IX-9 has a unique transient expression profile restricted to the bradyzoite, activation of which results in significantly decreased tissue cyst formation.

OR-02 **Kevin W. Petersen**[1], Andrea Lemus[1], Dr. James Leahy[1]
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Novel Synthesis of (+)-Catechin Metabolites

Catechin is a secondary metabolite that is present in most plants. This molecule belongs to the flavonoid class of antioxidant molecules and may be useful when researching diabetes and heart disease. When catechin is digested by animals, it is broken down into smaller molecules by the liver and intestines. These metabolites have been characterized, but their effects on animals are not fully well known. Researchers have demonstrated that some metabolites of catechin have properties against tissue inflammation. It is unknown whether these metabolites are targeting a specific enzyme. The goal of our research is to synthesize catechin metabolites so they can be externally evaluated to determine how they may be useful for diabetes pathways. The first target compounds are phenyl-gamma valerolactones that have never been synthesized without the use of microbes, therefore it is of great interest to find an alternative route of production for these compounds.

OR-03 **Nicholas Wallace**[1], Ankush Kanwar[1], James Leahy[1]
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Studies aimed at the Synthesis of Anti-malarial Agents

Malaria is a mosquito-borne disease caused by protozoan parasites of the Plasmodium genus. It is the fourth leading cause of death in the world, and is prevalent in lesser-developed countries. During its life cycle, there are two hosts including the mosquito and the mammal. Infected mammalian hosts contain the mature sexual stage, also known as gametocytes, of this parasite. In the gut lumen of the infected mosquitos, gametogenesis and the formation of diploid zygotes occurs. Xanthurenic acid (XA) is a tryptophan metabolite also present in the gut of the mosquito, and it has been shown to be the chemical trigger to induce gametogenesis. XA, as well as a series of analogs, have been synthesized with the goal of preventing the transmission of malaria and determining the biological mechanism responsible for this chemical signaling pathway.

OR-04 **Luciano Laratelli**[1]**, Vincent Roth**[1], Zachary Shultz[1], James Leahy[1]
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Progress Towards an Enantioselective Total Synthesis of the Membranolides

Membranolides are terpenoid natural products isolated from the Antarctic sea sponge, Dendrilla membranosa. Membranolide A and D had been shown to inhibit the growth of S. aureus and L. donovani in initial biological screens. The absolute stereochemistry and mode of action are currently unknown for the membranolides. An asymmetric total synthesis is under investigation to elucidate the absolute configuration and further explore the membranolides as anti-infective agents. Multiple routes have been explored incorporating a variety of Claisen rearrangements for stereocontrol of a challenging quaternary center. These routes and challenges faced will be discussed.

OR-05 **Ronald Swonger**[1], Andrea Lemus[1], James Leahy[1]
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Synthesis of Pentamidine Analogs as Potential Treatments of Leishmaniasis

Leishmaniasis is a disease caused by protozoan parasites of the genus Leishmania and is transmitted by the bite of an infected sandfly. There are roughly two million new cases a year, most of which occur in less developed countries around the world. Visceral leishmaniasis is the deadliest type with possible symptoms that include fever, anemia, weight loss, and organ enlargement. The current treatments of leishmaniasis

are toxic and expensive. Pentamidine is a drug used in certain cases of leishmaniasis, although it has toxic effects. The mechanism of action of pentamidine is currently unknown. In this lab, we have worked on synthesizing compounds using pentamidine as the framework for new analogs. Pentamidine contains a simple structure and we hope to make analogs quickly and efficiently. It is our hope that these compounds can show improved activity and better pharmacokinetic properties compared to pentamidine.

OR-06 **Sri Harsha Palakurty**[1,2], **David Herrera-Perez**[1,2], Linda Barbeto[1,2], James Leahy[1,2]
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Novel synthesis of SNX-2112 analog for Anti-leishmaniasis activity

Leishmaniasis is an infectious disease caused by species of the protozoan parasite Leishmania donovani. It is transmitted through the bite of the phlebotimine sandflies. SNX-2112 is a heat shock protein 90 (Hsp90) inhibitor that has been shown to be active in human cancer cells. It has shown promise in inhibiting the growth of multiple myeloma. In a high throughput screening campaign, we found that SNX-2112 is also active against Leishmania donovani. Chaperone proteins are believed to be critical to protozoans, so selective inhibition should inhibit the further replication of the parasite. Our target compound 1 is similar to SNX-2112 with the exception of a cyclopropyl group in the position of dimethyl. It is hypothesized that the change to a more rigid analog will lead to an improved activity/selectivity profile. Upon completion of the synthesis, we will assay 1 to evaluate its antiinfective and Hsp90 activity.

OR-07 **Melissa Chin**[1], Benjamin Eduful[1], James Leahy[1], David Kang[1]
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Targeting the SSH1 Protein Aimed at Reversal of β-amyloid Peptides Related to Alzheimer's Disease

Alzheimer's Disease (AD) is a progressive neurodegenerative disease for which there is no known cure. Currently, in the United States alone, there are more than 3000 cases of AD per year. AD is characterized by a buildup of β-amyloid peptides (Aβ's), leading to plaque formation in the brain and subsequent cognitive impairment. David Kang of the Byrd Institute has identified a protein known as Slingshot, SSH1, and has related it to the formation of Aβ's. Due to recent molecular modeling and docking studies, a molecule of the chemotype 2-pyridone-3-carboxylic acid has been shown to be significantly active against SSH1. Modeling suggests that the thiazole nitrogen forms hydrogen bonds with the Arg399 residues on SSH1. Therefore, analogs that increase or decrease this interaction will significantly impact biological activity. One such analog was synthesized and its activity against SSH1 was tested using various biological assays.

OR-08 **Holly Chery**[1]
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Synthesis and antibacterial activities of sulfenylated benzylpenicillin against Methicillin-resistant Staphylococcus aureus (MRSA)

Increasing the bioactivity of benzylpenicillin against Methicillin-resistant Staphylococcus aureus (MRSA) would have tremendous impact on treatment for infected patient. A potential approach is the modification of the secondary amide in benzylpenicillin. The acetylated benzylpenicillin as predicted was found to have no bioactivity in comparison to the non-modified Benzylpenicillin against (MRSA). The research goal is to sulfenylate Benzylpenicillin in order to increase its bioactivity against MRSA . The last step of reaction synthesis is the sulfenylation of Benzylpenicillin after the deprotection of the secondary amide. The crude product was obtained and purification process is still in progress. The sulfenylated benzylpenicillin will be investigated further in order to determine its bioactivity against MRSA. Modifying the secondary amide in benzylpenicillin can drastic effect on its bioactivity, we suggest that further research on this site may lead to the discovery of potent antibacterial against (MRSA).

OR-09 **Alexander Beard**[1], Faeez Mahzamani[1], Edward Turos[1]
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The Bioactivity Study of Antibiotic Loaded Chiral Polymer Nanoparticle Emulsions

The purpose of this investigation is to determine the effect of chirality on the efficacy of antibiotic nanoparticle emulsions against certain bacteria. The bacteria to be used in this testing are an antibiotic sensitive strain of Staphylococcus aureus and an antibiotic resistant strain of S. aureus (MRSA). This is important because of the prevalence of MRSA as the cause of hospital-borne infections. This investigation will determine the minimum inhibitory concentration against S. aureus and MRSA of D-menthol and L-menthol polymers loaded with variable amounts of penicillin-G. This will be compared to the bioactivity of penicillin-G to determine if there is a greater effect, and whether or not the chirality of the polymer itself has any effect.

OR-10 **Rubens Petit Hommes**[1], Deborah Bromfield Lee[1]
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Development of a green multi-week synthesis for the organic lab: Total synthesis towards calarene

Environmental concerns in the 1970's led to the increase in the significance of green chemistry, which peaked in the 1990's. Both industry and academia have been splicing some emphasis on organic reactions that can be performed more efficiently, safely and preventing unnecessary

waste. Calarene is a sesquiterpenes from the carene family, which was synthesized by Coates and Shaw in 1970. This project focuses on the development of greener synthesis of Calarene with comparison to established methods, using primarily reactions traditionally learned in Organic Chemistry, such as the Wittig and Diels Alder reactions. These reactions have been chosen because they utilize concepts tied to the 12 –principles of green chemistry. Additionally, the lab provides experience towards a total synthesis of a small molecule.

OR-11 **Grant Lawrence**[1,2], Zach Schultz[1,2], James Leahy[1,2]
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Progress Toward an Enantioselective Synthesis of the Cannabinoids and Analogs Utilizing the Claisen Rearrangement

Endocannabinoids, such as arachidonic acid, are known to inhibit the growth of the parasite Naegleria fowleri, a highly lethal brain eating amoeba. We envision that the cannabinoids from the cannabis plant could be a useful therapeutic for this parasite and potentially for a wide range of other therapeutic purposes. We are currently developing a novel synthesis of cannabinoids, such as THC and CBD, which allows for a variety of diversity to be introduced. Using Claisen Rearrangements, the two important stereocenters would be controlled with high enantioselectivity. This synthetic route should allow for the synthesis of a wide variety of cannabinoid analogs that will be screened against the parasite, as well as other therapeutic benefits.

PC-01 **Carrie Robart**[1], Fiona Kearns[1], Michael Kemp[1], Sai Lakshmana[1], H. Lee Woodcock[1]
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Boron-Nitrogen Dative Bonding Benchmark Analysis Using Computational Simulations

Recent studies with chemosenors utilize a boron-nitrogen interaction as the active sensing component. Computational simulations were used to analyze the structures of certain sensors to determine which sensor structure was lowest in energy. Gas phase calculations were run using QM/MM with different basis-set and functional pairs. Out of twenty isomeric forms of dimethylamine boronic acid fructose compounds, one structure, (5R,8R,9R,10S)-2(2((dimethylammonio)methyl)phenyl)-2,8,9,10-tetrahydroxy-1,3,6-trioxa-2-boraspiro[4.5]decan-2-uide, designated as structure b, was found to be most favorable in the system. The best basis set and functional pair for dative bonding from the gas phase at this point in the research is shown to be omegaB97x-D and 6-311++G**. Solvent phase calculations will also be conducted using QM/MM and CHARMM in an explicit water environment. All calculations will be compared to experimental results to determine what structure is most likely and what basis-set/functional pair is best at treating the boron-nitrogen interaction.

PC-02 **Corbin Rodier**[1], **Andres Saez**[1], **Devin Thorton**[1]
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Comparison of Models of Free Energy Landscapes by Overdamped Diffusion and Kinetic Models

We investigate the efficacy of two computational models – an overdamped diffusion model and a kinetic analysis model – in calculating the free energy landscape of dynamical systems. We test the two models on two systems: a protein driven from equilibrium and allowed to relax stochastically, and the Lorenz attractor. The two systems were simulated for long-term time intervals and compared to equilibrium dynamics. These are known for the protein system, and may be estimated for the Lorenz attractor. While both methods give an accurate picture of the free energy landscape of a system, the overdamped diffusion model by nature contains more noise, but is directly applicable to systems with unknown parameters. The kinetic model gives more accurate results by virtue of being deterministic, the system parameters must also be known. Between the models, a high-level, coarse-grained understanding of the behavior of dynamical systems (e.g. protein folding, enzyme activity) may be elucidated.

PC-03 **Joshua DeWeese**[1]
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Novel Production of Polyimide Thin Films via Electrospinning

Polymer physics began and continues to stay on the forefront of industrial application and technological innovation. A common class of polymers known as polyimides has shown to have a well-defined set of thermoplastic properties including: high thermal stability, high electrostatic resistivity, high tensile strength, as well as a high flame resistance. By using a material processing method known as Electrospinning, polymer fibers can be drawn out of solution via electrostatic force onto a grounded receiver. The fibers can vary from nanometer to micrometer length, with varying fiber diameter and bulk density. Electrospinning was used to produce fibrous thin films of a polyimide synthesized from Pyromellitic dianhydride, 3,3'5,5'-Tetramethyl-4,4'-diaminodiphenylmethane, and Jeffamine® polyetheramine. The resulting spun fibers have a white fibrous bulk texture with a morphology unique to the characterized length and concentration of the polyimide.

About the Cover

Spider dragline silk possesses exceptional mechanical properties, being lighter than Kevlar and having a tensile strength exceeding steel. This unique combination of extensibility and strength has promising applications in numerous fields, including artificial ligaments and tendons, as well as ultra-lightweight body armor. Despite this, there is little structural information available, and artificially produced silk is unable to capture many of the desirable characteristics of the naturally occurring counterpart. The cover image shows a structure of part of MASp1, one of two proteins found in dragline silk. This structure was obtained using temperature replica exchange molecular dynamics and provides further insight into the structural features of silk at the molecular level.