Raymond N. Castle Student Research Conference

13th

April 11, 2015

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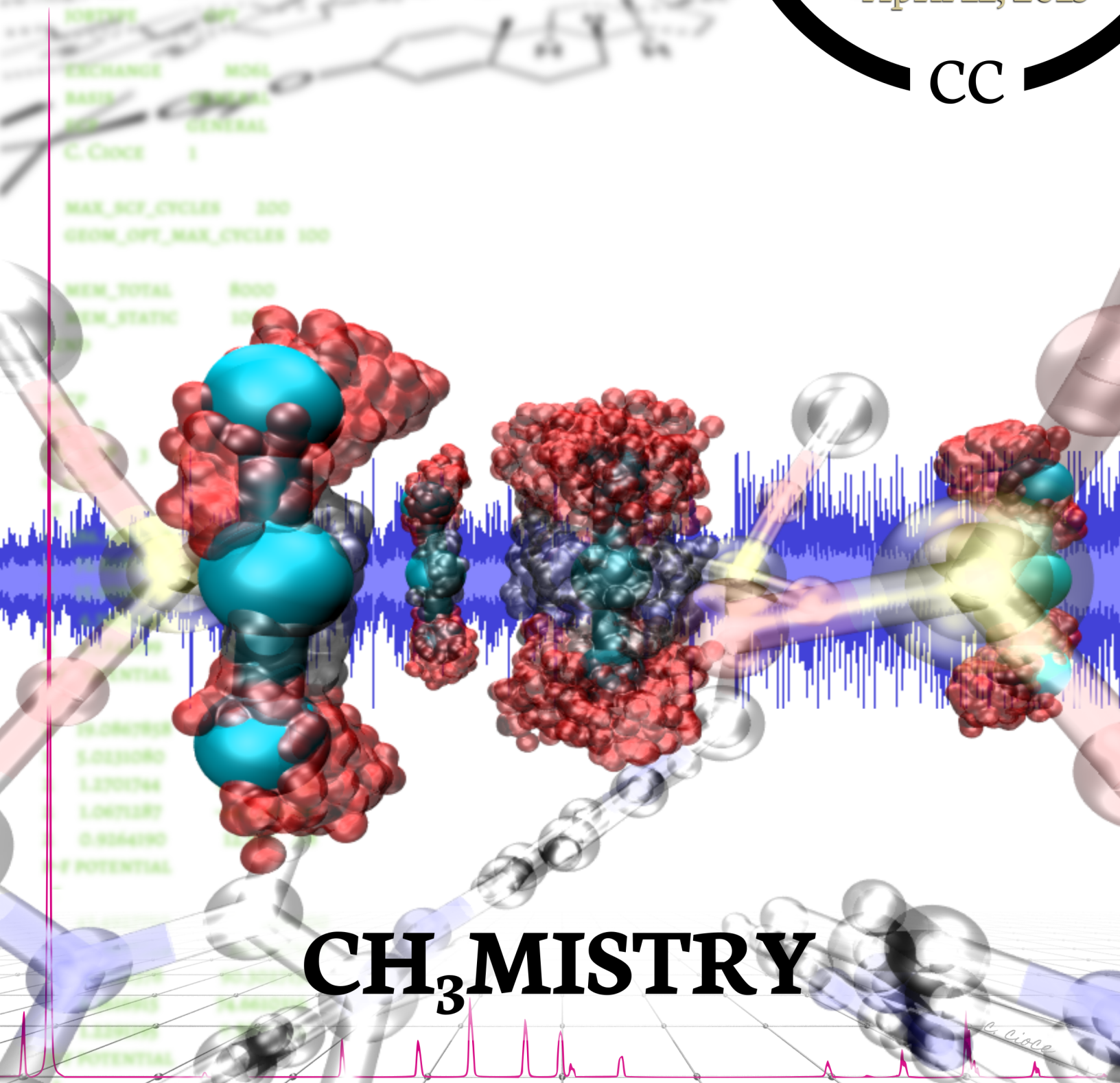

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University of South Florida
Department of Chemistry
4202 East Fowler Ave., CHE205
Tampa, FL 33620

13th Raymond N. Castle Student Research Conference

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Welcome from the Castle Conference Committee

Dear Colleagues and Friends,

Welcome to the 13th 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. Ingrid Montes. 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. Montes 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. Harmon 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 13th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

13th Raymond N. Castle Student Research Conference Committee

Committee Members

Darrell Cole Cerrato (Chair)
Jennifer Borja (Co-Chair)
Dan Utic
Kia Williams
Justin White
Alekhya Nimmagadda
Catherine Costa
Margarita Vanegas
Marie Bourgeois, PhD

Faculty Advisor

Julie Harmon, PhD

Staff & Faculty Support

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Carissa Vetromile, PhD
Edward Turos, PhD

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Brant Tudor

Program Cover Design

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Specials Thanks

Linda Lowe
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13th Raymond N. Castle Student Research Judges

University of South Florida

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Kirpal Bisht, PhD
Jianfeng Cai, PhD
Kathy Carvalho-Knighton, PhD
Daniel Cruz-Ramirez de Arellano, PhD
Xin Cui, PhD
Kimberly Fields, PhD
Jhon Figueroa, PhD
Ioannis Gelis, PhD
Joseph Gill, PhD
Ushiri Kulatunga, PhD
Mohan Kumar, PhD
Wayne Guida, PhD
Julie Harmon, PhD
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Shengqian Ma, PhD
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St. Leo University

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University of Central Florida

Alaa Hashim, PhD
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Ya Yuan, PhD

H. Lee Moffitt Cancer Center & Research Institute

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Florida Southern College

Deborah Bromfield Lee, PhD
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Tampa Chapter ACS Members

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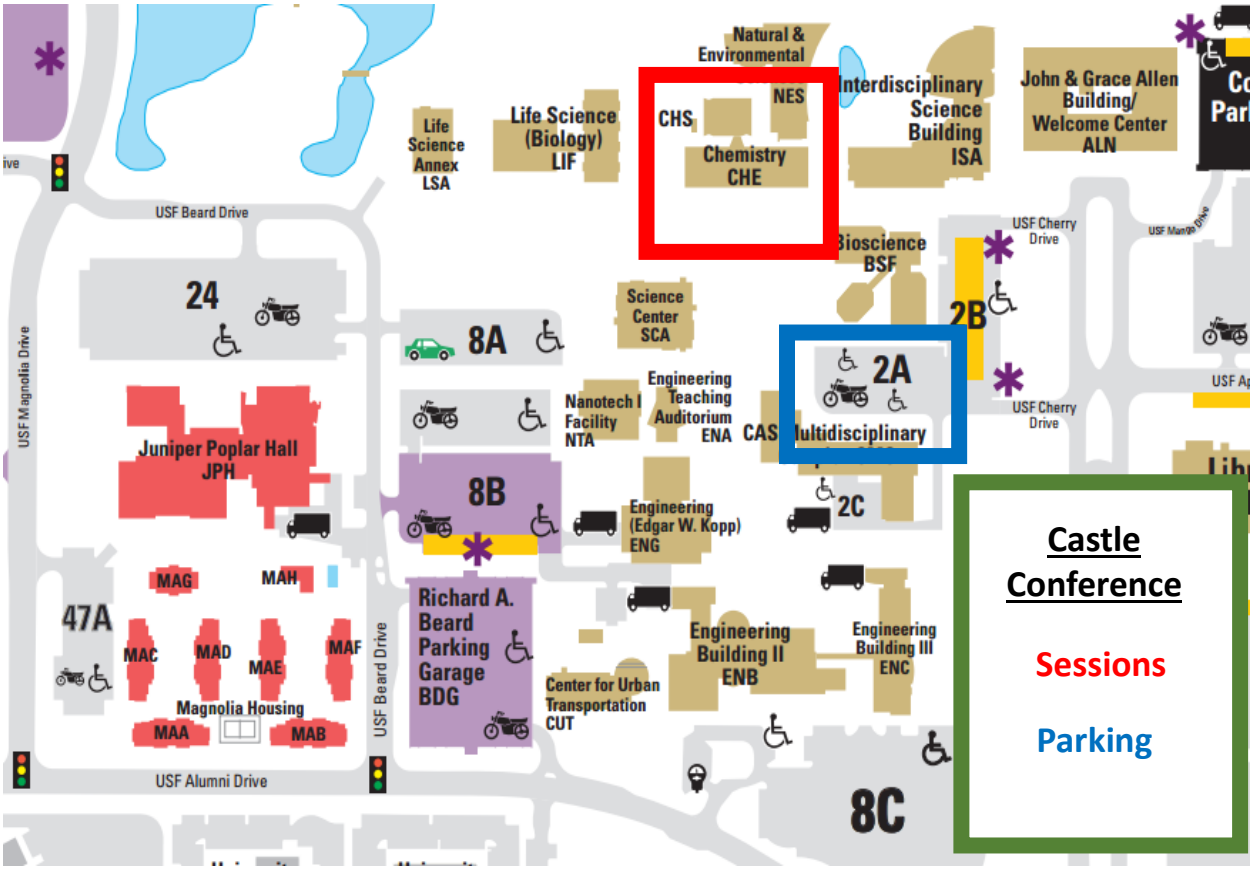
Sujeewa Ranatunga, PhD
Eric Johnson, PhD

Building Map



Schedule of Events

Saturday, April 11, 2015

8:00 AM	-	9:00 AM	**Welcome Session** - *Registration and Breakfast*	Chemistry Courtyard
9:00 AM	-	10:30 AM	**Morning Talk Sessions I & II** *Graduate Student Presentations*	CHE 100 & CHE 111
10:30 AM	-	10:45 AM	**Break**	
10:45 AM	-	11:00 AM	**Castle Conference Welcome**	CHE 100
11:00 AM	-	12:00 PM	**Plenary Speaker - Dr. Ingrid Montes**	CHE 100
12:00 PM	-	1:00 PM	**Lunch** *Sponsored by Tampa Chapter ACS*	Chemistry Courtyard
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	-	4:45 PM	**Afternoon Talk Sessions I & II** *Graduate Student Presentations*	CHE 100 & CHE 111
4:45 PM	-	5:00 PM	**Break**	
5:00 PM	-	5:15 PM	**Awards Ceremony**	CHE 100

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. Ingrid Montes
Plenary Speaker

Ingrid Montes received a B.S. in Chemistry and a Ph.D. in Organic Chemistry from the University of Puerto Rico at Río Piedras. She has taught chemistry at this Institution for 29 years, earning Full Professorship and tenure in 1998. Dr. Montes has two areas of current research: Organometallic chemistry and Chemical education. In the organometallic chemistry area, she explores the synthesis and characterization of various ferrocene derivatives and studies their potential applications in drug design, as redox-sensors and as polymers. She develops new methodologies in applying green chemistry principles. In education, her research is based upon the theoretical perspective, building on constructivist learning theory, mostly applied to organic chemistry, green chemistry and history of chemistry learning.

As a long-term educator, her philosophy is to assist students in their career development by encouraging networking, teamwork, effective communication, and critical thinking. In addition to this role, she believes strongly in the development of students' character and leadership by encouraging strong work ethics, service awareness and building self-esteem and self-insight. Together, this combination and foundation helps instill and inspire integrity, and an overall better technical professional.

For the past 25 years, Dr. Montes has been the Faculty Advisor of the ACS Student Affiliate (now, Student Member) Chapter. This chapter has received 22 consecutive ACS Student Outstanding Awards and has been recognized as Green Chapter a since its establishment. These positions have enabled her to mentor and inspire thousands of students, particularly Hispanic women.

Dr. Montes has been extremely active at the national, state and local level of chemistry in the roles of leadership, governance, and programming. She is Director-at-Large, Board of Director American Chemical Society ACS. She was Chair of the Theme Team for the ACS International Year of Chemistry (2011); Chair of the ACS Committee on Community Activities; Chair of the Advisory Board for ChemMatters Magazine; and a member of the Society Committee on Chemical Education (SOCED), among others. Dr. Montes was a member of the IUPAC 2011 Organizing Committee, including Chair of their Outreach Committee for 2011 Meeting held in Puerto Rico. At a local level she had been a member of the Board of Directors of the ACS-Puerto Rico Section for 20 years, where her roles have included Chair (1995, 2003, 2011) and Councilor (1998 to present). Additionally, she chairs the system wide committee of the University of Puerto Rico that oversees the improvement of academic chemistry programs.

Dr. Montes is an American Chemical Society and IUPAC (International Pure and Applied Chemistry) Fellow; she deserved the 2012 ACS Volunteer Service Award, received the ACS-Puerto Rico Section Leonardo Igaravidez Award; and ACS-Puerto Rico Section Chemical Education Award, among others.

Dr. Montes is an author/co-author of six laboratory manuals for teaching chemistry, over 200 presentations (co-authored with her students), and nearly 20-refereed publications over her distinguished career as both an educator

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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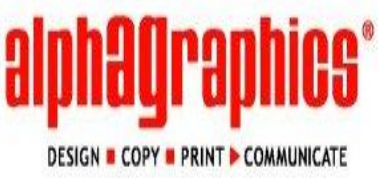

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Graduate Talks Morning Session I (CHE 100)

Session Chair: Dan Utic

9:00- 9:15 AM **Chris Witowski**

Ecological and Antileishmanial Activity of Diterpenoids Derived from the Antarctic Sponge Dendrilla membranosa

9:15- 9:30 AM **Danielle Demers**

New Antimicrobials from an Epigenetics Based Fungal Metabolite Screening Program

9:30- 9:45 AM **Haifan Wu**

New helical foldamers based on sulfono-gamma-AApeptides

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

10:00- 10:15 AM **Benjamin Eduful**

Synthesis of Novel Class of Anti-Leishmaniasis Agents

10:15- 10:30 AM **Walter Gonzalez**

Allosteric network in the neuronal calcium sensor protein DREAM

Graduate Talks Morning Session II (CHE 111)

Session Chair: Marie Bourgeois, PhD

9:00-9:15 AM **Jennifer Borja**

New Derivatives of N-Alkythio B Lactams New Multiimodal Functionality Impedes MRSA

9:15-9:30 AM **Jingyi Wang**

Highly Stereoselective Radical Cyclopropanation of Alkenes with Unsymmetric Diazomalonates via Cobalt(II)-Based Metalloradical Catalysis

9:30-9:45 AM **Tony Pham**

A Metal–Organic Material Platform Based Upon Alternating 4- and 6-connected Nodes

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

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1,2-Hydrogen Atom Transfer of α-Alkyl-α-diazoacetates via Cobalt(II)-based Metalloradical Catalysis

10:15-10:30 AM **Sreya Mukherjee**

Novel inhibitors of cruzain

Graduate Talks Afternoon Session I (CHE 100)

Session Chair: Kia Williams

3:15- 3:30 PM **Ha Thi Hoang Nguyen**

Ferulic acid and p-coumaric acid-based copolymers as biorenewable polyethylene terephthalate and polystyrene mimics

3:30- 3:45 PM **Khanh Ha**

Long-Range Intramolecular S to N Acyl Migration: a Study of the Formation of Native Peptide

3:45- 4:00 PM **Ning Ma**

DNA bend and base flip: possible trigger for UVDDB recognition process

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

4:15- 4:30 PM **Ken Kull**

Synthesis and Characterization of novel flexible polyimide containing long and short polyetheramine units

4:30- 4:45 PM **Arthur Maknenko**

Monitoring Guest-Host Interactions via Pulsed Field Gradient Diffusion NMR

Graduate Talks Afternoon Session II (CHE 111)

Session Chair: Alekhya Nimmagadda

3:15- 3:30 PM **Ashleigh Bachman**

The Biomimicry of Heme-Containing Peptoids: A Comparative Study against the Model Peptide Microperoxidase-11

3:30- 3:45 AM **Geoffrey M. Gray**

Temperature Replica Exchange Simulations of Major Ampullate Spidroin 1

3:45- 4:00 PM **Break**

4:00- 4:15 PM **Adam Hogan**

Developing the Next Generation of Classical Force Fields for Molecular Simulations

4:15- 4:30 PM **Alfredo Peguero-Tejada**

Endocrine-Disrupting Compounds: Exploring Solutions to Environmental Pollution

4:30-4:45 PM **Phillip Hudson**

QM Non-Boltzmann Bennett: A novel approach to ensure relevant sampling in free energy simulation based on energetic overlap between levels of theory

The Barbara and Dean F. Martin Poster Session
CHE 103
Session Chair: Marie Bourgeois, PhD

Graduate:	Group GP	All Disciplines

The Clear Springs Land Poster Session
CHE 101
Session Chair: Christie Tang

Undergraduate:	Analytical (AN), Biochemistry (BC), Biophysical (BP), Computational (CO), Inorganic (IN)

Tampa Chapter ACS Poster Session
CHE 101A
Session Chair: Siqi Sun

Undergraduate:	Organic (OR), Natural Products (NP)

GRADUATE TALKS

GT-01 **Chris Witowski**[1,2], Jackie von Salm[1,2], Alan Maschek[3], Brian Vesely[3], Dennis Kyle[3], Bill Baker[1,2]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery & Innovation, University of South Florida
[3]Department of Global Health, University of South Florida

Ecological and Antileishmanial Activity of Diterpenoids Derived from the Antarctic Sponge Dendrilla membranosa

The cold waters of Antarctica harbor bountiful marine life and biodiversity that promotes competition and the biosynthesis of defensive secondary metabolites. One inhabitant, the vibrant yellow sponge *Dendrilla membranosa*, is known to inhibit feeding of Antarctic predators such as sea stars and amphipods. A metabolomics approach was undertaken to identify whether sponges within the amphipod-rich algal canopy adopt different chemical profiles to account for the increased predation pressure. In addition, our group has identified the membranolides from *D. membranosa* that possess potent and selective activity against the leishmaniasis-causing parasite Leishmania donovani. The origin of these compounds will be investigated as artifacts from methanolic degradation of aplysulphurin.

GT-02 **Danielle Demers**[1,2], Lindsay Vacca, Renee Fleeman[3], Brian Vesely[3], Ala Azhari[3], Ashley Souza[3], Dennis E. Kyle[3], Lindsey N. Shaw[3], Bill J. Baker[1,2]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery & Innovation, University of South Florida
[3]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida

New Antimicrobials from an Epigenetics Based Fungal Metabolite Screening Program

Chemically diverse and largely under-studied, mangrove endophytic fungi represent a valuable source of natural products for a drug discovery screening program. While classical lab fermentation techniques may not reveal the full chemical potential of these organisms, epigenetic modification can encourage their full biosynthetic capabilities to be realized. As part of two NIH funded screening projects, mangrove endophytic fungi were grown under control and epigenetically modified conditions, extracted, and submitted for biological assay against a panel of the drug resistant and clinically relevant ESKAPE pathogens as well as against the tropical disease causing parasite Leishmania donovani. Active extracts were dereplicated, scaled up, and the compounds responsible for the activity were isolated and characterized. The investigation of one organism identified in this way yielded a suite of new, antimicrobial Cylindrols.

GT-03 **Haifan Wu**[1], Qiao Qiao, Jianfeng Cai
[1]Department of Chemistry, University of South Florida

New helical foldamers based on sulfono-gamma-AApeptides

Peptidomimetics are synthetic oligomers that resemble the activities of peptides. Their advantages over peptides include high stability towards proteolysis and enormous chemical diversity. Over the past two decades, there have been extensive efforts to develop peptide mimics, such as beta-peptides, peptoids, D-peptides, etc. The research on peptidomimetics have led to many important applications in both medicinal and material science. Here, we report the structural study of a new type of peptidomimetics, sulfono-gamma-AApeptides, by two-dimentional NMR and circular dichroism (CD) spectroscopy. The study suggests that sulfono-gamma-AApeptides adopt stable helical conformation in methanol, similar to alpha-helix structure. This finding will allow us to rationally design helical mimics that can be used to target protein-protein interfaces.

GT-04 **Benjamin Eduful**[1], Catherine Costa[2], Dennis Kyle[4], Brian Vesely[4], Tina Mukta[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Public Health, University of South Florida
[3]Department of Global Health, University of South Florida

Synthesis of Novel Class of Anti-Leishmaniasis Agents

Leishmaniasis is a parasitic disease transmitted through the bite of an infected female phlebotomine Sandfly. It is the 9th greatest disease burden among infectious diseases, but it is also classified as neglected tropical disease (NTD). Prevalent in developing countries, the disease presents in three main forms: Cutaneous (most common); Visceral (most severe form) and Mucocutaneous (most destructive form) Leishmaniasis. No vaccine currently exist but Antimony, Amphotericin or Pentamidine are used as treatments for the disease and none is particularly effective and are also associated with toxicity; hence the need to develop highly effective new drugs. It is known that Heat Shock Protein 90 (Hsp90) is one of the most abundant proteins in the protozoan parasite that causes Leishmaniasis; being involved in a variety of morphological processes. Inhibiting Hsp90 is therefore recognized as a potential therapeutic target. To this end, we are currently synthesizing novel Hsp90 inhibitors based on an unprecedented

GT-05 **Walter Gonzalez[1],** Jaroslava Miksovska[1]
[1]Department of Chemistry and Biochemistry, Florida International University

Allosteric network in the neuronal calcium sensor protein DREAM

DREAM/KChIP3 is a calcium-sensing protein that coassembles with Kv4 potassium channels in the brain and heart as well as with DNA in the nucleus where it regulates gene expression. The interaction of DREAM/KChIP3 with A-type Kv4 channels and DNA has been shown to regulate excitable cells. Previous results have shown a Ca^{2+} dependent interaction between DREAM/KChIP3 and Kv4/DNA which involves interactions at the N-terminus. In this work we propose that a highly conserved network of aromatic residues controls protein dynamics and the pathways of signal transduction on DREAM/KChIP3. Molecular dynamics simulations, site-directed mutagenesis and fluorescence spectroscopy provide strong evidence in support of a highly dynamics mechanism of signal transduction and regulation. Highlighting Tyr174 and Trp169 at the entering helix of EF-hand 3 as key amino acids involved in propagation of Ca^{2+} signals. This work provides the first mechanism of intramolecular signal transduction in a Ca^{2+} binding protein.

GT-06 **Jennifer Borja** Biplob Bhattacharya, Edward Turos[1]
[1]University of South Florida

New Derivatives of N-Alkythio B Lactams New Multiimodal Functionality Impedes MRSA

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. These derivatives of N-alkylthiolated -lactams are multimodal anti-MRSA bacteriostatic agents which inhibits Fatty Acid- biosynthesis.

GT-07 **Jingyi Wang[1]**, Xue Xu[1], Shifa Zhu[1], Xin Cui[1], Lukasz Wojtas[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Highly Stereoselective Radical Cyclopropanation of Alkenes with Unsymmetric Diazomalonates via Cobalt(II)-Based Metalloradical Catalysis

Cobalt(II)-based D2-symmetric chiral amidoporphyrin is able to enantioselectively perform a radical cyclopropanation with various types of alkenes and unsymmetric diazomalonates to afford asymmetric 1,1-diestercyclopropanes. The broad range of alkenes examined includes functionalized styrenes, such as halogen- or nitro- substituted styrenes, conjugated olefins, vinyl-substituted heterocycles, vinyl esters and acrylates. This cyclopropanation reaction undergoes a radical stepwise mechanism, in which Co(II) initiates the catalytic cycle with diazomalonate and then, with addition of olefin, radical migrates to the γ carbon and instantaneously cycles back to form a three-membered ring. The product, 1,1-diestercyclopane, is one kind of well-known synthon in organic synthesis. It can undergo a wide scope of ring-opening and cycloaddition reactions with various types of nucleophiles, reveal enormous potential as a versatile synthetic intermediate.

GT-08 **Tony Pham[1]**, Sameh K. Elsaidi[1,2], Mona H. Mohamed[1,3], Brian Space[1], Michael J. Zaworotko[1,3]
[1]Department of Chemistry, University of South Florida
[2]Chemistry Department, Faculty of Science, Alexandria University, Egypt
[3]Department of Chemical and Environmental Sciences, University of Limerick, Ireland

A Metal–Organic Material Platform Based Upon Alternating 4- and 6-connected Nodes

The fsc (four six type c) metal–organic material (MOM) platform is formed from alternating 4-connected $[Cu_2(CO_2R)_4]$ and 6-connected $[Cu(AN)_4]^{2+}$ (AN = aromatic nitrogen donor) moieties. Pore size control in this family of fsc MOMs was exerted by varying the length of the ligand, whereas pore chemistry was implemented using unsaturated metal centers (UMCs) and the use of either organic 1,5-napthalaenedisfulfonate (NDS) or inorganic SiF_6^{2-} ("SIFSIX") pillars. For MOMs that were synthesized using NDS, CO_2 sorption studies revealed higher isosteric heat of adsorption (Qst) for the material with the smallest pore sizes. In addition, using SIFSIX instead of NDS as a pillar resulted in eclipsed $[Cu_2(CO_2R)_4]$ moieties; the space between these moieties allows for a strong CO_2 binding site that can be regarded as an example of a single-molecule trap.

GT-09 **Sean Johnson[1]**, X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

1,2-Hydrogen Atom Transfer of α-Alkyl-α-diazoacetates via Cobalt(II)-based Metalloradical Catalysis

1,2-Hydrogen atom transfers are rarely observed in free-radical and organometallic chemistry. Through the use of cobalt(II)-based metalloradical catalysis this pathway was postulated for several α-alkyl-α-diazoacetates, generating never before studied β-Co(III)-alkyl radicals and yielding Z-selective acrylates. Using intermolecular hydrogen atom transfer probes, evidence supports the formation of β-Co(III)-alkyl radicals via isotopic labeling.

GT-10 **Sreya Mukherjee**[1], Wayne Guida[1]

Novel inhibitors of cruzain

Chagas' Disease, a parasitic disease caused by the parasite Trypanosma Cruzi, is endemic to Latin America. The disease manifests itself in a short acute phase and a long chronic phase. Current treatments are effective only in the acute phase and are not used in the chronic phase due to toxicity of the drugs. Hence a new drug discovery approach was chosen for this disease. Cruzain is the major etiologic enzyme involved in the disease and is only present in the parasite. It is also an enzyme expressed by the parasite in both phases. Herein, a novel virtual peptoid library containing known ketone based inhibitor was constructed and screened against cruzain. The peptoids thus found through this drug discovery effort can be used as potential drug candidates against cruzain. Computational techniques will help achieve a high degree of specificity and aid in proposing assays for determining compounds with high activity.

GT-11 **Ha Thi Hoang Nguyen**[1], Stephen A. Miller[1]
[1]Department of Chemistry, University of South Florida

Ferulic acid and p-coumaric acid-based copolymers as biorenewable polyethylene terephthalate and polystyrene mimics

Our goal is to synthesize polymers from abundant and inexpensive biorenewable monomers, yielding materials with thermal and mechanical properties which mimic or excel those of commodity polymers. Ferulic acid and p-coumaric acid, both naturally occurring hydroxycinnamic acids possessing antioxidant properties, derive from lignocellulose. They are used as starting materials to synthesize acetylferulic, acetyldihydroferulic, acetylcoumaric, and acetyldihydrocoumaric acid monomers. These monomers, when copolymerized at various feed ratios, produce copolymers with tunable thermal and physical properties. Some copolymers exhibit thermal properties comparable to commercially available non-renewable packaging plastics—particularly polyethylene terephthalate (PET) and polystyrene (PS). For example, the glass transition temperature can be tuned from 78 °C to 177 °C. With such promising properties, copolyesters from substituted hydroxycinnamic acids could prove to be sustainable replacements for non-biorenewable and non-degradable commodity plastics.

GP-12 **Khanh Ha**[1], Alan Katritzky[1]
[1]Department of Chemistry, University of Florida

S to N long-range acyl migrationstrategy for coupling of peptide fragments

Native chem. ligation (NCL), the most common form of chem. ligation, has become a widely used chemoselective technique to synthesize large peptides based on a capture/rearrangement concept. NCL has been extensively studied in peptidic compds. bearing a cysteine residue at the N terminus. Modified cysteine scaffolds have also been incorporated for the syntheses of novel peptides and proteins and for surface immobilization. The classical NCL method is limited to peptides possessing an N-terminal cysteine residue. To overcome this requirement of a specifically placed cysteine residue one approach is the use of thiol ligation auxiliaries, but unfortunately, removable cysteine mimics can sterically hinder ligation and difficulties can arise at the stage of auxiliary removal. We have successfully developed novel approach applying S to N long-range acyl migration to synthesize peptide and peptide analogs and also provided mechanistic evidence for the ligation process.

GT-13 **Ning Ma**[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

DNA bend and base flip: possible trigger for UVDDB recognition process

Ultraviolet light-induced pyrimidine photodimers are repaired by the nucleotide excision repair pathway, which is a sequence independent process. This damage introduces a kink and conformational change on DNA, which possibly activates the recognition process. After binding to DNA, the repair protein causes the damaged base to flip out, however the connection between the recognition of damaged DNA and DNA conformational change remains elusive. Here, we employed enhanced two-dimensional umbrella sampling computational method to uncover the link between the tendency of DNA to bend and flipping out of the damaged base, which may be important in the recognition process. Results indicate that damaged site increases DNA chain flexibility and bending, moreover it lowers the energy barrier for base flipping. That is most likely why the process like this is not observed for undamaged DNA.

GT-14 **Ken Kull**, Alejandro Rivera, Garrett Craft, Julianne Harmon
[1]Department of Chemistry, University of South Florida

Synthesis and Characterization of novel flexible polyimide containing long and short polyetheramine units

Polyimides are a class of high temperature resistant thermoplastic polymers that are most frequently used because of their thermal stability and good mechanical properties. A novel polyimide has been developed to solve the disadvantage of process-ability. The polyimide is composed of aromatic and aliphatic diamines to obtain the flexibility and rigidity optimal for the original purpose of solid state batteries. Different compositions of the diamines monomer are created to characterize the polymer and the different properties of it. Rheology, TGA, FTIR, Hardness and Tensile testing have been used to define the properties and characteristics of six different combinations. While the long aliphatic

chain reduces the thermal stability of the polymer, all of the compositions are above 98% stable up to 330ºC. The different lengths in the aliphatic chains provide a wide range for the manipulation of the Tg. Further studies need to be done to purify the polymer to narrow

GT-15 **Arthur Maknenko[1]**, Kirpal Bisht[1], and Edwin Rivera[1]
[1]Department of Chemistry, University of South Florida

Monitoring Guest-Host Interactions via Pulsed Field Gradient Diffusion NMR

Cyclodextrins (α, β, γ) are known to form complexes with a range of compounds, because their rigid cavity selects for either aliphatics, aromatics/heterocyles or even steroids. However, cyclodextrins are not equally abundant and cannot be selectively, chemically augmented. Resorcinarenes decorated with hydrophilic glucosides also form complexes in aqueous solutions, similar to cyclodextrins, but are changeable. Complexation of guests, DSS, Vanillin, Sunset Yellow FCF (SY) and hosts, β-cyclodextrin, CDR3 was monitored via Oneshot DOSY pulse sequence in D_2O at 23 ◦C.

GT-16 **Ashleigh Bachman**[1], Tarah A. Word[1], Randy W. Larsen[1]
[1]Department of Chemistry, University of South Florida

The Biomimicry of Heme-Containing Peptoids: A Comparative Study against the Model Peptide Microperoxidase-11

Peptoids are peptidomimetic oligomers composed of N-substituted glycine subunits that are highly valued for their convenient synthesis, superior cellular uptake, and resistance against enzymatic degradation. The unique structure of peptoids allows for the introduction of non-natural and diverse side chains, capable of generating extensive compound libraries with applications in drug discovery and material design. However, their successful biomimicry when synthesized in conjunction with a prosthetic heme group has yet to be explored. Herein, a comparison of the optical character and catalytic activity via an ABTS assay of the model heme-peptide microperoxidase-11 and its peptoid analogue is examined to ensure the structure and function of the synthetic peptidomimetic system is retained.

GT-17 **Geoffrey M. Gray[1]**, Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Temperature Replica Exchange Simulations of Major Ampullate Spidroin 1

While dragline silk is one of the strongest materials known, detailed insights into its structure are still lacking. Here we present temperature replica exchange simulations of major ampullate spidroin 1 mini-fibrils, a main component of the silk. A total of four systems was simulated, each with a different orientation of the crystalline polyalanine β-sheets. Our simulations showed the formation of 3-10 helices in the amorphous region, as well as the rearrangment of β-sheets in some of the systems. Comparisons to solid state NMR date will be made and implications of these structural features will be discussed.

GT-28 **Adam Hogan[1]**, Brian Space[1]
[1]Department of Chemistry, University of South Florida

Developing the Next Generation of Classical Force Fields for Molecular Simulations

Currently there is a pressing need to simulate a wide variety of molecules in the gas phase, the condensed phase, the bulk, in mixtures and in heterogeneous media. However, limitations in the accuracy, transferability and computational efficiency of current force fields have reduced their usefulness. These shortcomings will be addressed in this work by combining physically meaningful potential forms with high accuracy electronic structure calculations and benchmark thermodynamic data. The associated insights could have a significant impact in empirical force field modeling throughout science, including fields as diverse as liquids, polymers, solids, biology and soft matter.

GT-19 **Alfredo Peguero-Tejada[1]**, Aleksandra Karolak[1], Arjan van der Vaart[1]
[1]Department of Chemistry, University of South Florida

Enhanced sampling simulations of DNA 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. Test calculations on a large DNA data set showed that our simplified method achieves excellent correlation with 3DNA. We expect the method to be useful in quantifying base pair flexibilities from molecular dynamics free energy simulations.

GT-20 **Phillip Hudson**[1], Fiona Kearns[2], Gerhard König[3], Stefan Boresch[3], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida
[2]Laboratory of Computational Biology, National Institutes of Health
[3]Department of Computational Biological Chemistry, University of Vienna

QM Non-Boltzmann Bennett: A novel approach to ensure relevant sampling in free energy simulation based on energetic overlap between levels of theory

We have developed an accurate and efficient approach to free energy simulation that effectively calculates free energy by considering overlap between low and high level potential energy surfaces. The work presents benchmark results of the quantum mechanical non-Boltzmann Bennett method in calculation of solvation free energies and free energy profiles.

GRADUATE POSTERS

GP-01 **Brandon Welch**[1]
[1]Medical Technology, University of South Florida

Therapeutic effects of C-28 methyl ester of 2-cyano-3,12- dioxoolean-1,9-dien-28-oic acid (CDDO-Me)on radiation-induced lung inflammation and fibrosis

C-28 methyl ester of 2-Cyano-3,12- dioxoolean-1,9-dien-28-oic acid (CDDO-Me), one of the synthetic triterpenoids, has been found to have potent anti-inflammatory and anticancer properties in vitro and in vivo. However, its usefulness in mitigating radiation induced lung injury (RILI), including radiation induced lung inflammation and fibrosis, has not been tested. The aim of this study was to explore the therapeutic effect of CDDO-Me on RILI in mice and the underlying mechanisms. Herein, we found that administration of CDDO-Me improved histopathological score, reduced the number of inflammatory cells and concentrations of total protein in bronchoalveolar lavage fluid (BALF), suppressed secretion and expression of pro-inflammatory cytokines, including transforming growth factor-β (TGF-β) and interleukin (IL)-6, elevated the expression of anti-inflammatory cytokine IL-10, and down-regulated the mRNA level of pre-fibrotic genes, including fibronectin, α-smooth muscle actin (α-SMA), and collagen I. CDDO-Me attenuated radiation-induced lung inflammation. CDDO-Me also decreased the Masson's trichrome stain score, hydroxyproline content.

GP-02 **Matthew Battistini**[1], Chris Shoji[3], Sumit Handa[2], David Merkler[2]
[1]Institute for Environmental Chemistry, Department of Chemistry
[2]Department of Chemistry, University of South Florida
[3]Department of Chemistry, University of California, San Diego

Mechanistic Binding Insights for DXS, the Rate-Limiting Enzyme of Isoprenoid Biosynthesis in the Malaria-Causing Protists P. falciparum and P. vivax

Our lab has successfully truncated and recombinantly-expressed 1-deoxy-D-xylulose-5-phosphate Synthase (DXS) from both P. vivax and P. falciparum. We set about to elucidate the binding mechanism of this TPP-dependent enzyme using steady-state kinetic analyses, dead-end inhibition, and intrinsic tryptophan fluorescence titration. Both DXS enzymes adhere to a random sequential mechanism with respect to binding both substrates: pyruvate and D-glyceraldehyde-3-phosphate. This is in contrast to all other TPP-dependent enzymes which utilize a classical ping-pong mechanism. Our research will aid in the development of novel agents that target the non-mevalonate pathway of isoprenoid biosynthesis, which will help to treat malaria infection.

GP-03 **David Butcher**[1], Sophie Bernad[1], Pierre Sebban[1],Valerie Derriere[1], Jaroslava Miksovska[1]
[1]Department of Chemistry and Biochemistry, Florida International University
[2]Department of Chemistry & Physics, l'Université Paris-Sud

Role of ionic strength and the Bohr effect in modulating thermodynamic profiles associated with CO escape in rice non-symbiotic hemoglobin 1

Rice hemoglobin (rHb1) is a type 1 non-symbiotic hemoglobin belonging to the family of six-coordinated heme proteins which are found in all plants. Using photoacoustic calorimetry, we have characterized thermodynamic profiles for CO photorelease from wild type rHb1 and a distal histidine mutant. Under stripped conditions at pH 7.0, a temperature dependence of reaction volume and enthalpy change is observed. CO photo-release from the native protein below 16 °C is associated with ΔH of 29.3±2.3 kcal mol^{-1} and ΔV of 4.1 ± 0.3 mL mol^{-1}. Replacement of the distal histidine modifies the rate constant for CO rebinding however the thermodynamic profiles for CO escape are similar to those observed for the native protein. The addition of 500 mM NaCl or adjustment of the pH to 6.0 eliminates the observed temperature dependence. The impacts of electrostriction, Bohr effect, and protein oligomerization on observed values of ΔH and ΔV will be discussed.

GP-04 **Khoa Pham**[1], Jaroslava Miksovska[1]
[1]Department of Chemistry and Biochemistry, Florida International University

Identify the binding interface between DREAM and presenilin 1 C-terminal fragment

Interactions of downstream regulatory element antagonist modulator (DREAM) and presenilin-1 (PS1) are involved in several neuropathological processes. However, molecular details on the interaction interface between DREAM and PS1 as well as the impact of Ca^{2+}/Mg^{2+} on DREAM-PS1 complex formation remain unknown. Here, a combination of fluorescence steady-state anisotropy, fluorescence time-resolved anisotropy, stop-flow kinetics, and computational docking has been used to investigate the system. Titration data showed that Ca^{2+}DREAM binds to HL9 with a dissociation constant of 0.9 ± 0.1 μM and a 10-fold weaker affinity was determined for helix-7, whereas no interaction was observed for helix-β. Time-resolved anisotropy data indicate that Ca^{2+} DREAM interacts with PS1-HL9 in a dimeric form. The

high activation energy for Ca^{2+}DREAM association to HL9 (15.9 ± 3.1 kcal mol^{-1}) suggests conformational changes with decreased flexibility of the loop in DREAM upon interaction with HL9. The interaction interface between DREAM and PS1 will be discussed.

GP-05 **Douglas Franz[1]**, **Aaron Mohammed[1],** Katherine Forrest[1], Brian Space[1]
[1]Department of Chemistry, University of South Florida

Understanding gas-MOF interactions by calculation of relative atomic charges in novel MOF NOTT-112

Metal Organic Frameworks have been an object of a rapidly growing field of chemical research due to their wide range of application and almost limitless amount of designable structures. Of particular interest is their capacity to readily and quantitatively absorb gases. In this work, using x-ray diffraction data provided by experimental groups, charges of atoms in a single unit cell of NOTT-112, a novel copper based bimetallic center rht-MOF, were calculated by means of geometry optimization and charge potential calculations with NWCHEM to analyse the potential sorption capacities of the material for multiples gases. Particular attention is given to the nature of the bimetallic centers, whose copper atoms predictably have varying charges based on the conformation of the MOF structure, and thus different affinities to gaseous molecules.

GP-06 **Sreya Mukherjee[1]**, Wesley Brooks[1], Wayne Guida[1]
[1]Department of Chemistry, University of South Florida

Study of a transmembrane protein : STIM1

Calcium ions plays an important role in various physiological functions such as signaling, protein folding, enzyme activation and cell apoptosis. Stromal Interaction Molecule 1, STIM1 an ER transmembrane protein is activated by a drop in ER calcium levels and interacts with ORA1 a plasma membrane protein to form channels which then allows extracellular calcium ions to enter the cell and restore balance. Dysregulation of calcium flux has been reported in cancers, autoimmune diseases and other diseases with STIM1 being an interesting target in drug discovery due to its key role early in calcium flux. Herein, computational techniques was used to model a structure of the transmembrane protein and was mechanistic analysis was done on it to understand how the protein works which is overexpressed in various diseases.

GP-07 **Michael Veri[1]**
[1]Department of Chemistry, University of South Florida

Compound Isolation and Structural Elucidation From Marine Sources

Marine bacteria and invertebrates represent rich sources for novel chemistry. Metabolites produced by these organisms are already tailored to function in biological systems; as such, these chemicals are well-suited for use as drugs. A discovery program in the Baker Lab has already yielded compounds of interest, and more await discovery.

GP-08 **Matthew A Knestrick[1,2]**, Danielle H. Demers[1,2], Renee Fleeman[3], Lindsey N. Shaw[3], Bill J. Baker[1]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery & Innovation, University of South Florida
[3]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida

Epigenetic Modification of Tampa Bay Fungal Strain Produces New and Known Compounds Active Against MRSA

In the face of increasingly resistant bacteria like the ESKAPE pathogens, there is a dire need for new and novel drug candidates. Marine fungal endophytes live in harsh environments, producing secondary metabolites as a survival strategy. In the laboratory, production of secondary metabolites is often down-regulated. Epigenetic modifiers can be used to activate down regulated biosynthetic pathways to access a greater chemical repertoire. Following a high-throughput, epigenetic-based screen of mangrove endophytic fungi, one fungal strain from the Tampa Bay area was identified for its activity against ESKAPE pathogen Staphylococcus aureus. It was grown in large scale and in epigenetically modified conditions. Its secondary metabolites were extracted, and the fractionation and purification of extracts was guided by NMR. Epigenetic modification of the fungi caused the production of a suite of new and known compounds, with one derivative found only in the modified conditions exhibiting activity against S. aureus.

GP-9 **Elizabeth Yancey**[1,2], Renee Fleeman[3], Bill J Baker[1,2], Les N Shaw[4]
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery & Innovation, University of South Florida
[3]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida
Optimization of Fungal Metabolite Expression Via Epigenetic Modification For Drug Discovery

The harsh and competitive environment in which marine microbes live instigates their production of chemical defenses. When cultured, these environmental pressures are not present, leading to the down-regulation of some biosynthetic pathways. Artificial stressors are often applied to activate an enhanced metabolic response in the laboratory setting. For example, upon epigenetic modification, endophytic fungi from Floridian mangroves have been found to produce secondary metabolites not observed in untreated cultures, and to increase the number of fungal extracts found to be active in bioassay against virulent pathogens by about 50%. We have begun to study the effects potent, selective histone deacetylase (HDAC) inhibitors to determine what, if any, effect HDAC-specificity has on epigenetic control in coaxing secondary metabolites from cultured fungi. Metabolomics via LC/QToF MS has been employed to quantify the similarity of compound profiles produced by each modified fungal sample, and activity against the ESKAPE pathogens assessed.

GP-10 Marvin Duvalsaint[1], **Andrew J. Shilling** [2,3], Ryan M. Young[2,3], R. Kennedy Keller [4], Bill J. Baker[2,3], Dennis E. Kyle[4]
[1]College of Pharmacy, University of South Florida
[2]Department of Chemistry, University of South Florida
[3]Center for Drug Discovery & Innovation, University of South Florida
[4]Department of Global Health, University of South Florida

Total synthesis of 13C labelled isoprenol for the elucidation of the abscisic acid biosynthetic pathway in of the malaria parasite Plasmodium falcipar

The malaria parasite Plasmodium falciparum is theorized to undergo dormancy to escape stress from antimalarial treatments. Abscisic acid (ABA), a phytohormone involved in seed dormancy, may also play a key role in regulating this parasitic dormancy. We have detected ABA in the blood stages of *P. falciparum* and aim to characterize its biosynthesis utilizing 13C labelled metabolic ABA precursor, [13C] geranylgeranyl pyrophosphate (GGPP). In order to accomplish this, we must first carry out the total synthesis of [13C] isoprenol, which will be pyrophosphorylated to yield [13C] isopentenyl pyrophosphate (IPP) and then converted to [13C] GGPP by the enzyme GGPP synthase. The metabolic label will then be used to determine intermediates on the ABA pathway within the parasite. Our long-term goals will center on elucidating and understanding ABA's role in *P. falciparum*.

GP-11 **Yong Wang**[1], Xin Wen[1], Xin Cui[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Asymmetric Radical Cyclopropanation with in Situ Generated Donor-Substituted Diazo Reagents via Co(II)-Based Metalloradical Catalysis

Asymmetric radical cyclopropanation with in situ generated donor-substituted diazo reagents has been developed via Co(II)-based metalloradical catalysis. The cobalt(II) complex of D2-symmetric chiral porphyrin, 3,5-DitBu-Xu(2'-Naph)Phyrin, has proven to be an effective metalloradical catalyst for asymmetric cyclopropanation of a broad range of olefins with different N-arylsulfonyl hydrazones, affording the desired cyclopropane products in high yields with both excellent diastereoselectivity and enantioselectivity. This Co(II)-based metalloradical system renders a direct and effective protocol for the utilization of less stable donor-type diazo reagents and to achieve their asymmetric cyclopropanation transformations.

GP-12 **Lucas Parvin**[1], Xin Cui[1], Li-Mei Jin[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Enantioselective (4+1) Cycloaddition of 2-Siloxy-1,3-Dienes via Co(II)-Based Metalloradical Catalysis

Five-membered carbocycles are a type of important motif in both natural products and pharmaceutical compounds. For this reason, new methodology for the efficient synthesis of cyclopentane rings is desired. Co(II)-Based metalloradical catalysis has been proved to enable (4+1) cycloaddition of 2-ethyl-2-cyano-diazoacetate with 2-siloxy-1,3-butadienes through selective radical cascade. This method, which operates at room temperature, is able to construct a wide variety of multi-functionalized cyclopentene derivatives with good enantio- and diastereoselectivity, with nitrogen gas as the only byproduct.

GP-13 **Xin Wen**[1], Yong Wang[1], Xin Cui[1], Limei Jin[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Asymmetric Intramolecular C–H Alkylation of Sulfonylhydrazones as Precursors for Donor-Type Diazo Reagents via Co(II)-Based Metalloradical Catalysis

The Co(II) complex of D2-symmetric chiral porphyrin 2,6-DiMeOChenPhyrin, [Co(P3)], has been shown to be a highly effective metalloradical catalyst for asymmetric intramolecular C–H alkylation of sulfonylhydrazones as precursors for donor-substituted diazo reagent. The [Co(P3)]-catalyzed radical C–H alkylation is suitable to C–H bonds adjacent to a variety of aromatic functional groups with varied electronic and steric properties, providing the corresponding chiral 2,3-dihydrobenzofuran in high yields with good enantioselectivity.

GP-14 **Jingyi Wang**[1], Xue Xu[1], Shifa Zhu[1], Xin Cui[1], Lukasz Wojtas[1], X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

Highly Stereoselective Radical Cyclopropanation of Alkenes with Unsymmetric Diazomalonates via Cobalt(II)-Based Metalloradical Catalysis

Cobalt(II)-based D2-symmetric chiral amidoporphyrin is able to enantioselectively perform a radical cyclopropanation with various types of alkenes and unsymmetric diazomalonates to afford asymmetric 1,1-diestercyclopropanes. The broad range of alkenes examined includes functionalized styrenes, such as halogen- or nitro- substituted styrenes, conjugated olefins, vinyl-substituted heterocycles, vinyl esters and acrylates. This cyclopropanation reaction undergoes a radical stepwise mechanism, in which Co(II) initiates the catalytic cycle with diazomalonate and then, with addition of olefin, radical migrates to the γ carbon and instantaneously cycles back to form a three-membered ring. The product, 1,1-diestercyclopane, is one kind of well-known synthon in organic synthesis. It can undergo a wide scope of ring-opening and cycloaddition reactions with various types of nucleophiles, reveal enormous potential as a versatile synthetic intermediate.

GP-15 **Andrea Lemus**[1], Kevin Petersen[1], James W. Leahy[1]
[1]Department of Chemistry, University of South Florida

Novel Synthesis of (+)-Catechin Metabolites

Catechin is a compound of the flavan-3-ol family of plant secondary metabolites. It is metabolized into smaller molecules by the liver and intestines when ingested by animals. The specific functions of these metabolites are unknown, although this class of molecules has been shown to have anti-inflammatory properties and therefore could be useful for diabetes research. Some phenyl-gamma-valerolactones have been found to be effective superoxide scavengers and similar compounds have anticancer and neuroprotective properties. We wish to report our synthesis of two known catechin metabolites so that they can be further evaluated in an effort to determine how they might be useful in diabetes pathways. These compounds have never been synthesized before without the use of microbes, so it is of interest to find an alternative route that will provide useful quantities. The metabolites were synthesized racemic, although the route can be altered for enantioselective synthesis through a single step change.

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

Design and the Synthesis of pseudo-Cyclodextrin Resorcin[4]arenes (CDR's) and their Application in Thiocyanation Reactions in Water

Water-soluble pseudo-cyclodextrin resorcin[4]arenes (CDRs) were designed and synthesized by decorating the upper rim of synthesized resorcin[4]arene intermediates with β-D-glucopyranosyl moieties via Cu(I)-catalyzed Azide-Alkyne Cycloaddition (CuAAC). The utility of the CDRs was demonstrated as catalysts for eco-friendly thiocyanation reactions in water for water-insoluble alkyl/aryl bromides. The use of aqueous media in organic syntheses is of great importance, especially to limit the use of toxic and volatile organic solvents, particularly of the chlorinated hydrocarbons. The results show that a variety of alkyl and aryl bromide derivatives were well tolerated within 30 minutes and more than 90% conversions were observed; functionalities included unsaturation, carbonyl groups, esters and bromo lactones. The substitution of cyclic or acyclic secondary (20) bromide proceeded with equal ease. The ^{1}H-NMR investigation established the encapsulation of the benzyl thiocyanate inside the cavity of the CDRs.

GP-17 Jeanine Yacoub[1]
[1]Department of Chemistry, University of South Florida

Searching for drug targets and possible treatments for toxoplasmosis

Toxoplasmosis is a zoonotic disease caused by the protozoan parasite *Toxoplasma gondii*. Humans are infected most commonly from ingestion of uncooked meat of infected animals, or accidental ingestion or inhalation from cat feces. In immunocompromised patients, the infection could cause encephalitis and/or growth of brain masses. Current treatment for toxoplasmosis includes combinational drug therapy. However, patients suffer from problems of intolerance, allergic reactions, and an inability to cure the infection. In an effort to identify new kinase targets to treat this disease, we have been working on the synthesis of a series of compounds that can be used as tools to probe the unique pathways used *by T. gondii*. One such series are pyridinyl imidazoles, which have been shown to be active against MAP kinases.

GP-18 Edward Turos,[1,2], Lindsey Shaw[2], **Daniel Utic[1]**, Renee Fleeman[2]
[1]Department of Chemistry, University of South Florida
[2]Department of Integrative Biology, University of South Florida

High Throughput Screening of Synthetic Antibacterial Agents against ESKAPE pathogens.

Approximately 1000 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 agents included N-thiolated beta-lactams, new alkyl disulfide analogs, rifamycins, and other classes of drugs. Further studies will involve synthesis of the most active analogs as well as examination of resistance.

GP-19 **Sean Johnson[1]**, X. Peter Zhang[1]
[1]Department of Chemistry, University of South Florida

1,2-Hydrogen Atom Transfer of α-Alkyl-α-diazoacetates via Cobalt(II)-based Metalloradical Catalysis

1,2-Hydrogen atom transfers are rarely observed in free-radical and organometallic chemistry. Through the use of cobalt(II)-based metalloradical catalysis this pathway was postulated for several α-alkyl-α-diazoacetates, generating never before studied β-Co(III)-alkyl radicals and yielding Z-selective acrylates. Using intermolecular hydrogen atom transfer probes, evidence supports the formation of β-Co(III)-alkyl radicals via isotopic labeling.

GP-20 Ken Kull[1], **Alejandro Rivera[1]**
[1]Department of Chemistry, University of South Florida

Synthesis and Characterization of novel flexible polyimide containing long and short polyetheramine units

Polyimides are a class of high temperature resistant thermoplastic polymers that are most frequently used because of their thermal stability and good mechanical properties. A novel polyimide has been developed to solve the disadvantage of process-ability. The polyimide is composed of aromatic and aliphatic diamines to obtain the flexibility and rigidity optimal for the original purpose of battery application. Different compositions of the diamines monomer are created to characterize the polymer and the different properties of it. Rheology, TGA, FTIR, Hardness and Tensile testing have been used to define the properties and characteristics of six different combinations. While the long aliphatic chain reduces the thermal stability of the polymer, all of the compositions are above 98% stable up to 330ºC. The different lengths in the aliphatic chains provide a wide range for the manipulation of the Tg. Further studies need to be done to purify the polymer to narrow the molecular weight distribution and try composites to ameliorate its properties.

GP-21 **Tamalia Julien[1]** , Julie Harmon[1], Garrett Craft[1]
[1]Department of Chemistry, University of South Florida

Thermal and mechanical properties of thermoplastic polyurethanes incorporated with nanoparticles

Polycarbonate Polyurethanes (PCPU) are a family of thermoplastic polymers that are used in various biological and industrial applications. The ultra-soft PCPU formulation used in this project has the ability to reform its original shape after being stretched or damaged. Hydrogen bonding within the PCPU is thought to be primarily responsible for the mechanical characteristics and the manifestation of the observed self-healing properties. It has been shown that silver, silica and copper nanoparticles have multiple hydrogen bonding sites which can interact with the PCPU. The research undertaken includes adding one percent by weight of the silver and silica nanoparticles as well as copper-based paddle wheel $[Cu_2(p\text{-OH benzoate})_4(DMSO)_2]\bullet 2DMSO$ with the PCPU. The goal of this project is to see whether these nanoparticles improve the mechanical and thermal properties of the PCPU. Different techniques such as Differential Scanning Calorimetry, Tensile Testing, and FT-IR Spectroscopy, will be used.

GP-23 **Linda Barbeto**[1], James Leahy[1], Andrea Lemus[1], Alex Branton[1], Sri Palakurty[1], Dennis Kyle[2]
[1]Department of Chemistry, University of South Florida
[2]Department of Global Health, University of South Florida

Studies Aimed at the Synthesis of Alcohol-linked Hsp90 Inhibitors as Antileishmaniasis Agents

Visceral leishmaniasis is a parasitic disease prevalent in less developed countries for which no effective treatments are available. Studies have shown that compounds effective against Hsp90 are also active against Leishmania donovani cells. Our lab is currently investigating novel Hsp90 inhibitors with the goal of discovering new antileishmaniasis agents. Our project consists of making alcohol linked inhibitors in order to explore additional binding sites in the active site in an attempt to increase inhibition.

GP-24 **Garrett Craft**[1], Andrew Lopez[1]
[1]Department of Chemistry, University of South Florida

Rheological analysis of novel polyimide polymers

Novel polyimide polymers are characterized by rheology. Rheology is a sensitive oscillatory technique used to study the flow of matter either in liquid, solid or, more commonly, the viscoelastic state. Stress or strain applied in an oscillatory fashion at various frequencies probes the physical transitions and moduli of the material in question.

GP-25 **Phillip Hudson**[1], Fiona Kearns[2], Gerhard König[3], Stefan Boresch[3], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida
[2]Laboratory of Computational Biology, National Institutes of Health
[3]Department of Computational Biological Chemistry, University of Vienna

QM Non-Boltzmann Bennett: A novel approach to ensure relevant sampling in free energy simulation based on energetic overlap between levels of theory

We have developed an accurate and efficient approach to free energy simulation that effectively calculates free energy by considering overlap between low and high level potential energy surfaces. The work presents benchmark results of the quantum mechanical non-Boltzmann Bennett method in calculation of solvation free energies and free energy profiles.

UNDERGRADUATE POSTERS

AN-01**Tanya Sehgal**[1], Tarah A. Word[1], Dean F. Martin[1]
[1]Department of Chemistry, University of South Florida
Removal of pain-relieving drugs from aqueous solutions using Octolig® and selected metalloligs

Removing active pharmaceutical ingredients (API) from wastewater is important because it can reduce contamination of crops treated in wastewater. In this study Octolig® was used in order to remove pharmaceuticals from water, a commercially available material with polyethyldiamine moieties covalently attached to high-surface area silica gel. The two drugs used were acetaminophen and naproxen; they are commonly used for pain and fever reducing properties. These selected drugs were tested using column chromatography by removal of ion encapsulation. The effectiveness of this treatment depends on having the appropriate anionic functional group. Most APIs have a high solubility, in accordance with the Biopharmaceutics Classification System and thus form anionic species in waste water. The samples were run using the same conditions: 50mL aliquots were collected, flow rate of 10mL/min, and samples 4-10 were analyzed by recording absorbance values, pH, and TDS. Removal was effective for naproxen, (82%), less so for acetaminophen (51%).

AN-02 **Umberto Napoletano**[1], Jess Jones[1]
[1]School of Arts and Sciences, Saint Leo University

The use of ultrasound for the optimization of the SNAr reaction of piperidine and 1-fluoro-4-nitrobenzene

Sonochemistry takes advantage of ultrasonic waves for their ability to produce microscopic bubbles in solution that release extreme heat and pressure in a phenomenon named Acoustic Cavitation. The use of ultrasound to initiate nucleophilic aromatic substitution reactions have shown to increase product yield and purity, compared to reactions driven by heat. An ultrasonic cleaning bath (40 kHz, 110 W) was used to drive the reaction of 1-fluoro-4-nitrobenzene and piperidine to create 1-(4-nitrophenyl) piperidine. Initial reactions were conducted in DMSO under both thermal and ultrasonic conditions. The reaction was optimized by varying the solvents used, the ratios of the reagents, and the amount of time being exposed to ultrasonic conditions. The products have shown that the use of ultrasound indeed increases the yield and purity, compared to the heat driven reaction. The thermal reaction in DMSO produced a 27% yield, while the same reaction under ultrasonic conditions produced a 92% yield.

AN-03 **Vivian Lee**[1], Siqi Sun[1], Xiao Sheryl Li[1]
[1]Department of Chemistry, University of South Florida

Synthesis of Fe_3O_3@Ag Nanoparticles for Surface-Enhanced Raman Spectroscopy

Nanoparticles created employing magnetic and optical properties combined with noble metals show great potential for a variety of biological and environmental applications. The goal is to design a sensitive, rapid, and reliable pollutant detection method wherein Fe_3O_4@Ag nanoparticles produce high magnetization, uniform size, and high surface-enhanced Raman scattering (SERS) enhancement. Multiple synthesis methods were explored including the seed-growth method, water-in-oil microemulsion method, and interfacial self-assembly method. Uniformity of the nanoparticles were observed by transmission electron microcopy (TEM), optical properties were detected by UV-Vis and SERS, and sensitivity of SERS substrates were identified using a common SERS probe molecule rhodamine 6G. It was found the core-shell size of Fe_3O_4@Ag is tunable by adjusting the ratio of its constituents and plays a key importance in SERS signal enhancement. The results revealed for SERS detection, the optimum ratio between Fe_3O_4 and Ag_2SO_4 is 1:35, and the optimum concentration of Fe_3O_4@Ag is 5 mM.

AN-04 **Timothy Odom**[1], Mohanraja Kumar,[1] Haifan Wu,[1] Abdul Malik[1]
[1]Department of Chemistry, University of South Florida

Amylin Peptide Optimization: Synthesis and Characterization

This study was to find an optimized technique for the synthesis and purification of the peptide amylin. The peptide was developed using Fmoc solid phase peptide synthesis. The sequence of the peptide contained residues 26-37; three amino acids within the sequence were altered in order to assist with the solubility of the peptide during purification. The main focus of the study was to optimize the purification of the peptide through development of RP-HPLC conditions. These conditions included altering the HPLC mobile phase gradient and solutions used during purification. The peptide was characterized using LCMS to ensure the identity as well as CD to determine secondary structures. LCMS analysis of the crude product confirmed the synthesis of the peptide, and purification through HPLC was able to isolate the peptide from the crude mixture.

AN-05 Abdullah Alhendal[1]
[1]Department of Chemistry, University of South Florida

Zirconia-Based Sol-Gel Microextraction

Catecholamines and their acidic metabolites are known as biomarkers for neuroendocrine tumors such as neuroblastoma and pheochromocytoma. In this study, novel amphiphilic sol-gel zirconia-based organic-inorganic biocompatible sorbents will be developed in the form of a surface coating for the extraction and preconcentration of catecholamines and their acidic metabolites. Sol-gel zirconia (zirconium oxide, ZrO_2) based sorbents are introduced to overcome the drawbacks of the silica-based sorbents that are traditionally used for the detection and quantitation of catecholamines. Zirconia enhanced pH stability compared to the conventional silica-based materials. The many intermolecular interaction sites can enhance the sorption capabilities of the zirconia-based hybrid materials compared to silica-based or pure organic polymer-based counterparts. In this study, sol-gel technology will be used for the creation of polypropylene oxide (PPO)-based zirconia sorbents for capillary microextraction. Preliminary results showed a noticeable affinity toward catechol compared to its isomers, indicating promising performance for detection and quantification of biomarkers.

AN-06 **Skylyr Strader[1], Jess Jones[1]**
[1]Center for Drug Discovery & Innovation, University of South Florida
[2]School of Arts and Sciences, Saint Leo University

The examination of heavy metal ion concentrations and their relationship to albanism in propagules of Rhizophora mangle (Red mangroves) in Tampa Bay.

Rhizophora mangle are routinely affected by oil spills because of their location in coastal areas. In addition to the organic components, oil spills commonly have enriched levels of heavy metals. Polycyclic aromatic hydrocarbons have been linked to genetic mutations, but the PAHs are only one component of oil spills. A readily visible indicator of genetic mutations in mangroves are propagules exhibiting albinism. The concentrations of two metals: lead and copper, were compared in samples taken from locations of known frequencies of albinism to determine if a correlation is present. The locations being investigated are War Veterans Park, Simmons Park, Sawyer Key, and Elanore Island. These locations were chosen because of their documented histories of oil spills (excluding War Veterans Park) and their varying levels of albinism frequencies.

AN-07 Stan Stevens[1], Joao Costa Pinho[1], **Katherine Wissert[1]**
[1]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida

Propionylation and MS Analysis of EtOH-induced PTMs to Microglia

Ethanol consumption has wide-ranging impacts throughout the body. This study sought to compare histone post-translational modifications (PTMs) due to oxidative stress of mouse microglial cells with different levels of ethanol exposure. Analyzing PTMs via mass spectroscopy continues to be a challenge because the protease trypsin cleaves at lysine and arginine sites, and histones are rich in both amino acid residues. Propionylation, or treatment of histones with propionic anhydride, blocks lysine sites from trypsin digestion. This leads to more hydrophillic fragments which are better resolved using reverse-phase HPLC and mass spectra that are simpler to interpret. While propionylation has been utilized on other cell types, this is the first time it has been used to analyze microglial cells.

AN-08 **Stephanie Mengis, Jake Matthews,** Abdullah Alhendal
University of South Florida

Zirconia-Based Sol-Gel Microextraction

Catecholamines and their acidic metabolites are known as biomarkers for neuroendocrine tumors such as neuroblastoma and pheochromocytoma. In this study, novel amphiphilic sol-gel zirconia-based organic-inorganic biocompatible sorbents will be developed in the form of a surface coating for the extraction and preconcentration of catecholamines and their acidic metabolites. Sol-gel zirconia (zirconium oxide, ZrO2) based sorbents are introduced to overcome the drawbacks of the silica-based sorbents that are traditionally used for the detection and quantitation of catecholamines. Zirconia enhanced pH stability compared to the conventional silica-based materials. The many intermolecular interaction sites can enhance the sorption capabilities of the zirconia-based hybrid materials compared to silica-based or pure organic polymer-based counterparts. In this study, sol-gel technology will be used for the creation of polypropylene oxide (PPO)-based zirconia sorbents for capillary microextraction. Preliminary results showed a noticeable affinity toward catechol compared to its isomers, indicating promising performance for detection and quantification of biomarkers.

BC-01**Taylor Mitchell[1,2]**
[1]Department of Chemistry, University of South Florida
[2]Center for Drug Discovery & Innovation, University of South Florida

Improvement in Implementation of Polymer-Based Artificial Tissue to Aid in Tissue Regeneration

Variation of polymers impinges on the effectiveness of the artificial tissue scaffolding. Currently there is research comparing the benefits of polymers such as polylactides and polyglycolic acid. One must take into account the biodegradability, processability, and mechanical properties of such polymers. Although all are able to form an injectable gel composition, the ability of all polymers to achieve the mechanical and biodegradable properties necessary to promote regenerative growth is in question. I intend to utilize the research of other scientists to analyze variations in polymer-based artificial tissues and determine what attributes contribute to affective tissue regeneration. I will investigate variations in types of polymers used to form artificial tissues, the biocompatibility of polymers, as well as the role the polymer plays in the overall effectiveness of tissue regeneration. I hypothesize that the more hydrophilic and flexible the biocompatible material is, the better chance it has at being an effective material.

BC-02 **Sierra Teegarden**[1], Tamalia Julien[1], Julie Harmon[1]
[1]Department of Chemistry, University of South Florida

Strengthening Self-Healing Properties of Polycarbonate Polyurethane through the Addition of Nano Composites

The goal of this project is to compare the weights of nano-composites to self-healing abilities of Polycarbonate Polyurethane. This class of polymer has alternating soft and hard segments that allow for both flexibility and strength. PCPU has the ability for intrinsic self-healing after damage. Hydrogen bonding is thought to be the primary cause for the mechanical characteristics and self-healing properties observed. Nanosilver (WT: 30-50 nm) and nanosilica (WT: 20 nm) composites have multiple hydrogen bonding sites that the polar PCPU can interact with. A weight percentage of 0.5% was used for each composite except for nano-silica, which a 10% weight percentage was used because there were no significant findings in the 0.5% sample. Techniques such as Differential Scanning Calorimetry, Tensile Testing, FTIR Spectroscopy, and healing analysis will be used to analyze the composites' thermal, mechanical, and optical properties, how they relate and change with composition, and how they affect the self-healing ability of the neat polymer.

BC-03 **Jenny Mojarena Martin**[1], Tarah A. Word[1], Dean F. Martin[1]
[1]Department of Chemistry, University of South Florida

Removal of aqueous samples of selected NSAIDs (non-steroidal anti-inflammatory drugs) by Octolig®

Pharmaceutical drugs are organic or inorganic compounds used in the diagnosis, cure, treatment, or prevention of disease. Pharmaceuticals uses include veterinary, plant pharmaceuticals, or even illicit drugs. [2] One category of pharmaceuticals, of special interest to us, is NSAIDs. The working hypothesis is that Octolig® has the capacity to remove anionic species through attraction to protonated nitrogen. Dichlorfenac was of interest because the compound has significant veterinary uses. Briefly, a Spectra/chron peristaltic pump was used to deliver aqueous samples to a CHEMGLASS chromatography column. The column was packed with about a known volume of Octolig® . The effect of column volume was investigated and the results show a progressive improvement in the percentage removal for columns packed with greater amounts, specifically for 44 mL Octolig® (77.7±2%, 83.9±1.7% removal), 62 mL (83.9±1.7%, 87.3±5.7%) and 125 mL (90.5 ±2.8). Additional compounds are under investigation, including Indomethacin.

BC-04 **Paige Cooke**[1], Jiazhi Sun[2]
[1]Department of Chemistry, University of South Florida
[2]College of Pharmacy, University of South Florida

Repurposing of the FDA-approved anti-cancer tyrosine kinase inhibitor (dasatinib)

Dasatinib is an oral drug also known as Sprycel, discovered by Jagaandhu Das. It is a tyrosine kinase inhibitor (TKI) and has been approved for the treatment of patients with chronic myelogenous leukemia (CML) and a specified type of acute lymphoblastic leukemia (ALL). We hypothesize that this TKIs acts on other molecular targets in addition to tyrosine kinases that work together to regulate a number of important cellular processes. Employing the comprehensive docking method with our established chemical protein interactome (CPI) and 11 FDA-approved TKIs, we have discovered 301 PDB-deposited proteins corresponding. Dasatinib-CPI docking results show TKI-off-target interaction. The top 8 off-targets were EGFR, HDAC7A, BRAF, PPAR-Y, GPCR (A2AR), VDR, p53, Hsp90, and FTase. EGFR was the primary target. The systemic pharmacology approach validated the molecular targets of TKIs in vitro and efficacy study in vivo. Cell flow cytometry data showed induced apoptosis from the TKI.

BC-05 **Devon Marshall**[1], **Amit Dudhat,** Dimitra Keramasinou[1], Ioannis Gelis[1]
[1]Department of Chemistry, University of South Florida

Assembly mechanism of cochaperone-kinase complexes

Cdc37 is a cochaperone that functions as the gatekeeper for kinase entry into the Hsp90 chaperone cycle. It is implicated to cancer initiation and progression due to its association with proto-oncogenic client kinases and their recruitment to Hsp90. Our goal is to study the mechanism behind the selectivity that Cdc37 displays for Hsp90-dependent kinases over Hsp90-independent kinases. Previous structural methods used to resolve the structure of Cdc37-kinase complexes have been unsuccessful due to the dynamic nature and low conformational stability of the substrates. In order to gain a high resolution insight to the specificity determinants involved in differentiating Hsp90-dependent and Hsp90-independent kinases, as well as to be able to further elucidate the structure of Cdc37, we have employed nuclear magnetic resonance spectroscopy (NMR) in combination with isothermal titration calorimetry (ITC). Our studies reveal the specificity determinants embedded within the chaperone that orchestrates sorting and entry of oncogenic substrates into the Hsp90 chaperone cycle. They also form the basis for the rational design of novel anti-cancer drugs targeting Cdc37-substrate complex formation.

BC-06 **Victoria Ramos**[1], Walter G. Gonzalez[1], Jaroslava Miksovska[1]
[1]Department of Chemistry and Biochemistry, Florida International University

Characterization of the photophysical, thermodynamic and structural properties of the Terbium (III)-KChIP3 complex.

The focus of our research is to better understand the binding mechanism and structural changes that DREAM undergoes upon binding of Ca2+. To this end we employed terbium(III) as a calcium biomimetic and characterized its interaction with DREAM using thermodynamic and spectroscopic techniques. Using circular dichroism, temperature stability, fluorescence spectroscopy and isothermal calorimetry we were able to show that terbium(III) bound DREAM forms an intermediate structure that exposes hydrophobic cavities. Terbium(III) binding to CaM and DREAM show identical thermodynamics but the induced structural changes are different. The relevance of these findings not only expands the knowledge of the calcium and terbium binding properties of neuronal calcium sensors but also provides insight on how these proteins regulate heart pacemaking and neuronal signaling.

BC-07 **Arti Patel**[1], Toni-Ann Lewis[2], Malathi Narayan[3], Prachi Shukla[1], Jeana Ortiz[1], Umesh Jinwal[2]
[1]Department of Chemistry, University of South Florida
[2]Department of Pharmaceutical Sciences, College of Pharmacy, University of South Florida
[3]Byrd Alzheimer's Institute, University of South Florida

Effect of Cdc37 on the C-terminal TDP43 expressing C. elegans

The aggregation of the C-terminal kDa(C25) fragment of Trans-active response DNA binding protein (TDP43), is linked to neurodegenerative diseases such as Amyotrophic Lateral Sclerosis and Frontotemporal Dementia. Our cell based data showed Cdc37, a chaperone protein, plays a major role in the regulation of TDP43 and other proteins. We aimed to determine the effect Cdc37 has on behavior and aging, of wild type and C25-TDP43 expressing *C. elegans* animal models. We have generated transgenic Cdc37-expressing *C. elegans* and crossed it with the C25-TDP43 expressing *C.elegans*. Wild type, transgenic, and hybrid *C. elegans* models were analyzed to determine aging and behavior using life span and liquid thrash assays, respectively. Preliminary data suggests that Cdc37 has a profound effect on behavior and aging of C25 *C. elegans.*

BC-08 **Bryan MacNeill**[1], Marc Lajeunesse[1]
[1]Department of Integrative Biology, University of South Florida

Can river flow mechanics and hydro-chemical differences drive variation in parasitism of anchovies by isopods?

A river's flow regime and water chemistry are important drivers of many ecosystem components. However, few studies explore how differences in flow rates and water chemistry among rivers can influence communities of parasites and their hosts. Here, we investigated the impact of flow mechanics and different hydro-chemical components between Alafia and Hillsborough Rivers on the prevalence and intensity of natatory-isopod parasites (*Livoneca ovailis*) of the Bay Anchovy (*Anchoa mitchili*). We also explored seasonality in parasitism by comparing monthly samples from the two rivers throughout 2005-2008. We found that anchovies from Alafia River had a significantly higher intensity and prevalence of parasitism than those from Hillsborough; however strong seasonality in the abundance of anchovies in both rivers was also an important predictor of parasitic infections. Our results suggest that the higher flow rate and lower chemical concentrations of the Alafia River may provide more opportunities for parasites to infect hosts.

BC-09 **Keishla Rodríguez Graciani**[1], Raúl Alenó[1], Marco Miranda[1,] Joan Delgado Irizarry[1] Eulalia Medina[1], Lourdes Díaz Figueroa[1], Edmy J. Ferrer Torres*.[1]
[1]Department of Science and Technology, Inter American University of Puerto Rico, Ponce Campus, Mercedita, and P.R. 00715. *Research Director, ejferrer@ponce.inter.edu

Antimicrobial effect of improved antibiotics combined with Ni and Semi-Green Ag nanoparticles in Klebsiella pneumoniae

Bacterial resistance to antimicrobial agents is a major problem worldwide. The daily increase of resistant strains can trigger a variety of infections. Nanotechnology offers possible alternative treatments, improving the antimicrobial activity of antibiotics, due to the properties of different metals. Our main objective is to develop more effective treatments against these resistant bacterial and nosocomial infections, combining metal nanoparticles with antibiotics. In this study, two different nanoparticles, Ni and Semi Green Ag, were combined with antibiotics. The antibiotics Penicillin, Amoxicillin, Levofloxacin and Vancomycin, were used at two different concentrations against *Klebsiella pneumoniae* (ATCC # 13882), the causal agent of pneumonia and urinary tract infections in humans. Also, it revealed the antimicrobial effects of determined concentrations of antibiotics and nanoparticles, at equal and different proportions, against the bacteria. The results showed that some nanoparticles mixed with the antibiotics, at specific concentrations, increased the potential activity of the antibiotic against the bacteria, while in others the nanoparticles mixed with the antibiotics decreased the potential activity of the antibiotics.

BC-10 Maldonado Vélez Gabriel[1], Medina-Pérez Eulalia[1], Osorio Cantillo Celia[1], Ramírez-Domenech José I.[1]and Ferrer-Torres Edmy J[1].
-Department of Sciences & Technology, Inter American University of Puerto Rico, Ponce Campus, 104 Turpeaux Ind Park, Mercedita PR 00715-1602

Functionalization of Indole-3-Acetic Acid with gold nanoparticles synthesized through a double reduction reaction using leaflets' extracts of Leucaena leucocephala *(Lam.) de Witt.*

The chemical profile of *Leucaena leucocephala*, a worldwide distributed mimosoid legume, is suitable to explore its role in the synthesis of nanoparticles and their functionalization with organic molecules such as plant hormones. Functionalization of plant hormones with nanoparticles is an innovative strategy to enhance the impact of nanotechnology in environmental stress situations and biotechnology. In this work gold nanoparticles were synthesized making a double reduction using leaflets' extracts of *L. leucocephala* and citrate. The obtained nanoparticles were characterized, using a UV spectroscopy and a Dynamic light scattering to estimate the nanoparticle size. Results of green gold nanoparticles functionalized with hormone Indole-3-Acetic Acid shows a red shift displacement at 545-572 nm, indicating functionalization. The nanoparticle remained stable for four weeks and the size ranged between 65-80 nm. These results indicate the effectiveness of the *Leucaena* leaflets' extracts in the synthesis and functionalization of the gold nanoparticles.

BP-01 **Michael Jaquier**[1]
[1]Department of Chemistry, University of South Florida

M-Domain relaxation studies via NMR

NMR provides an invaluable tool for the analysis of protein dynamics and relaxation times. Abstraction of these data provide insight into protein function with an ultimate goal of ascertaining potential treatment options for a myriad of diseases. This study determines the dynamics and relaxation of the M-Domain of a protein identified as a critical functional component of cancerous cells.

BP-02 **Tabitha Alain Michau**[1]
[1]College of Public Health, University of South Florida

Predicting the Post-Operative Development of Right Ventricular Dysfunction in Patients implanted with a Left Ventricular Assistance Device

Other studies and analysis done within the field have looked at comparative effects of continuous flow LVADs to pulsatile LVADs as the standard of care option, or have been a comprehensive meta-analysis of this topic. Further, other studies have only analyzed the pre-operative confounding variables that could contribute to RVD following LVAD implantation; therefore leaving a gap in the knowledge of what other variables could be contributing factors to a pre-emptive prediction of post-operatively development with RVD. In order to fill the gap of knowledge, this study looked to investigate how preoperative, as well as intraoperative and immediate postoperative clinical variables may lead to the development of right ventricular dysfunction (RVD) following continuous-flow left ventricular assistance device (axial CF-LVAD) implantation. This study seeks to anticipate what patients will demonstrate early indications for the need for BIVAD support, as opposed to isolated LVAD support.

BP-03 **Andres Arango**[1], Walter G. Gonzalez[1], Jaroslava Miksovska[1]
[1]Department of Chemistry and Biochemistry, Florida International University

Insight into the calmodulin and DREAM protein complex interaction, mechanism and function

DREAM (Downstream-regulatory-element-antagonistic-modulator) is a neuronal calcium sensor which modulates gene expression. We show that association of calcium calmodulin (CaM) with DREAM is mediated by an amino-acid sequence on residues 29-44 of DREAM. The association of CaM with a peptide DREAM(29-44) or to native DREAM is calcium dependent (KD of 136 nM and 3.4μM, respectively). Thermodynamic/kinetic studies show the decreased affinity of native protein is due to electrostatic interaction between the basic N-terminus and an acidic surface on DREAM. Fluorescence-anisotropy decay measurements showed rotational-correlation times of 10.8 ns for CaM:DREAM(29-44), supporting a wraparound-semispherical model. Interactions between IEDANS labeled CaM with DREAM are best modeled as heterotetramers. Calcium CaM:DREAM adopts an elongated conformation (correlation time 45 ns). Additionally, CaM:DREAM association eliminates nonspecific interaction of DREAM with the DRE-dsDNA sequence of human prodynorphin gene. The presented work provides a molecular insight into CaM:DREAM and its potential role in modulation of gene expression.

BP-04 **Ashleigh Bachman**[1], Tarah Word[1], Randy Larsen[1]
[1]Department of Chemistry, University of South Florida

The Biomimicry of Heme-Containing Peptoids: A Comparative Study against the Model Peptide Microperoxidase-11

Peptoids are peptidomimetic oligomers composed of N-substituted glycine subunits that are highly valued for their convenient synthesis, superior cellular uptake, and resistance against enzymatic degradation. The unique structure of peptoids allows for the introduction of non-natural and diverse side chains, capable of generating extensive compound libraries with applications in drug discovery and material design. However, their successful biomimicry when synthesized in conjunction with a prosthetic heme group has yet to be explored. Herein, a comparison of the optical character and catalytic activity via an ABTS assay of the model heme-peptide microperoxidase-11 and its peptoid analogue is examined to ensure the structure and function of the synthetic peptidomimetic system is retained.

BP-05 **Ramirez Santiago, Lenianne**[1] , López Collazo, Anthony[1], Ramírez Domenech Jose[1], Osorio Cantillo, Celia[1] and Ferrer Torres, Edmy J.[1] ejferrer@ponce.inter.edu
1.Science and Technology Department, Interamerican University of Puerto Rico, Mercedita, Puerto Rico, United States.

Comparative study and characterization of MgO, ZnO AND CuO nanoparticles using amino acids as capping agents.

Synthesis of ZnO, MgO and CuO nanoparticles was done using sonochemical method. Colloidal and powder nanoparticles were obtained using zinc sulfate hydrate, magnesium chloride and copper sulfate as zinc, magnesium and copper sources respectively. Tetramethyl ammonium was employed as a surfactant. Polyvinyl Alcohol (PVA) and Polyethileneglycol (PEG) were used as stabilizers. Characterization, following synthesis, was done using optical spectroscopy (Ultraviolet Spectroscopy), Infrared Spectroscopy (FT-IR) and Diffracted Light Scattering (DLS). Kinetics studies were done to further information on nucleation and growth. These studies include changes in: reactants concentrations, sonication time and titration rate and heating time. Optical studies show the formation of the clusters and the nanostructures. The size of the nanoparticles was obtained using DLS. The size distribution was 34nm for ZnO, 68nm for MgO and 14nm for CuO. The absorption bands for the nanostructures formation were centered in 358 nm for ZnO nanoparticles, 600 nm for CuO nanoparticles and 335 nm for MgO nanoparticles. The ZnO nanoparticles and MgO nanoparticles was stabilized using cysteine and methionine amino acids. New studies using CuO and lysine was performed.

BP-06 Marco A. Miranda Belandria[1], Marangelie Feliciano Sanchez[1], Pedro Rivera Pomales[1], Eulalia Medina[1], Jose I. Ramirez Domenech[1], Celia Osorio Cantillo[1], Edmy J. Ferrer Torres[1]
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Functionalization and characterization of bimetallic silver-gold nanoparticles with antibiotics

New methods for drugs detections are necessary to improve the time and sensitivity for drug testing. Our work is focused in the development of a strategy to produce bimetallic silver-gold core-shell nanoparticles for the study of drugs interactions. Formation of the nanoparticles was achieved by the reduction of the AgNO3 with NaBH4 and HAuCl4 with sodium citrate and polyethylene glycol. A conventional microwave was applied to complete the synthesis. This technology offers minimization of reaction times and stabilization of nanoparticles. In this research, we explore the interactions with Penicillin, Ciprofloxacin, Vancomycin and Clindamycin with the silver-gold core shell nanoparticles. Characterization of the nanoparticles was performed using UV-Vis absorption spectroscopy with a band absorption center at 523 nm, Diffracted Light Scattering (DLS) study shows a mean diameter of 75 nm. Interaction with antibiotics results in a red shift between 15-70 nm. Also a change in color is produced with the addition of the antibiotics to the bimetallic nanoparticles.

CE-01 **Razanne Oueini[1]**, **Austin Dickerson[1]**, Razanne Oueini[1], Li Ye[1], Scott Lewis[1]
[1]Department of Chemistry, University of South Florida

Using text messages to understand student study habits and their relationship to success in General Chemistry

Efforts to improve student success in learning chemistry can benefit by a greater understanding of how students' study. Studying is defined here as any outside-of-class activities intended to promote success in an academic subject. Student study activities were collected through self-report in response to text message queries. Over 300 General Chemistry I students who voluntarily participated in this study were sent the text message "Have you studied General Chemistry I in the past 48 hours? If so, how?" at random intervals throughout the academic term, averaging approximately two messages per week. This poster will present the frequency and variety of student study habits in General Chemistry I and the relation between study habits and academic success as determined by in-class test scores.

CE-02 **Megan Gower[1]**, Benjamin Brittain[1]
[1]Department of Math and Science, Saint Leo University

History of Chemistry in chemical education: Social and chemical catalysts in the Multiple Discovery of hormone herbicides

Multiple Discoveries (MDs) facilitate integration of History of Chemistry (HoC) in chemistry courses. Chemistry MDs occur when scientists independently propose a theory or discover similar chemical substances, phenomena, or processes. MDs theories are related to discovery and creativity; therefore relevant to chemists. The heroic theory relies on agency of geniuses whereas sociological accounts emphasize social factors as catalysts for discoveries. This study explores the role of HoC and MDs in chemistry education and presents an in-depth historical case study: discovery of hormone herbicides. It uses systematic search and analysis of HoC and MDs literature in top-tier chemistry education journals (1963-2015) and content analysis of a Chemistry textbook. MDs are non-existent in chemistry education literature. Sixteen articles found related to HoC. Textbook references to HoC were scant (mode: 2.5/chapter), superficial, void of pedagogical value, and perpetuated the genius perception of discoverers. In contrast, the case study overwhelmingly supports the sociological account.

CE-03 **Ishan Chopra[1]**, Matthew Chrzanowski[1], **Romel Pancho[1], John O'Connor[1]**, Santiago Sandi-Urena[1]
[1]Department of Chemistry, University of South Florida

Reform in general chemistry laboratory instruction: How do students experience change?

Laboratory instruction has potential of developing fundamental science practices; however, little evidence supports its realization. Evidence collected, mostly quantitative, focuses on satisfaction and performance, comparing students in different learning environments. This qualitative inquiry investigates the experience of a cohort exposed to two substantially different laboratory environments. The focus on change of laboratory format renders complementary understanding to that from participants who experienced a single format. The first semester was a traditional expository program. The following semester was a cooperative, problem-based, multi-week format. Eleven students were interviewed individually after their completion of the sequence. A phenomenology was used for the reduction, analysis, and interpretation of data. The study identified several vectors of change served as lens to analyze the phenomenon. The participants experienced the transition from mindlessness to mindfulness. This experience was independent of participants' approval/disapproval. This work informs the design of laboratory experiences furthering the potential realization of experimental education.

CE-04 **Marwa Elkharsity[1]**, Dean Martin[1]
[1]Department of Chemistry, University of South Florida

Chemist at War

Chemists at war: World War II roles of five chemists. MARWA ELKHARSITY and DEAN F. MARTIN. Typically we recognize that chemists are involved in industry, academe, and government service, but it seems appropriate to examine the activities of chemists in times of political crises, such as wartime. In this poster we consider the activities of five chemists during World War I, e.g.,Roger Adams (University of Illinois), Robert Alldredge (DuPont), W. Conard Fernelius (Purdue), Frank Whitmore (Penn State), and Jonas Kamlet (Kamlet Laboratories). The greatest emphasis is given to Jonas Kamlet because of the availability of information in his personal and professional papers at USF.

CE-05 **Ben Brittain[1]**, Meagan Gower[1]
[1]Department of Chemistry, University of South Florida

Attribution of Boyle-Mariotte gas law discovery: a case study of Multiple Discoveries in chemistry education

Multiple Discoveries (MDs) occur when chemists independently propose a theory or discover similar chemical substances, phenomena, or processes. MDs are relevant to practicing chemists since they relate to scientific discovery and creativity. Scientists hold a heroic view of discovery that supports the agency of individual geniuses over sociological accounts emphasizing social factors as catalysts for discoveries. This study explores use of HoC and MDs in chemistry education and presents an in-depth historical case study: attribution of the Boyles-

Mariotte Gas Law. This work uses systematic search and analysis of HoC and MDs literature in top-tier chemistry education journals (1963-2015) and content analysis of a General Chemistry textbook. MDs are non-existent in chemistry education literature. Sixteen articles found related to HoC. Textbook references to HoC were scant (mode: 2.5/chapter), superficial, void of pedagogical value, and perpetuated the genius perception of discoverers. In contrast, the case study overwhelmingly supports the sociological account.

CO-01 **Fiona Kearns**[1], Sai Lakshmana Vankayala[1], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida

How does catalase release nitric oxide? Elucidating the reaction mechanism with QM/MM

Hydroxyurea (HU) is currently the only FDA approved treatment for sickle cell disease (SCD) and it is known to affect symptom relief by interacting with blood borne heme enzymes, like catalase, which convert HU to NO. It is our goal in this work to use computational techniques (molecular dynamics and quantum mechanical/molecular mechanical) to predict the most likely reaction pathway for the release of NO by catalase. Thus far, a model for catalase compound I has been constructed using CHARMM, and quantum mechanically optimized geometries have been attained using QChem as well as we have found the reactant complex to be in the doublet spin state. Additionally, we have performed initial screening analysis of the PubChem Database to identify a library of possible NO releasing substrates (HU analogs). Work continues in using reaction mapping techniques to predict the most likely reaction mechanism by which catalase converts HU to NO.

CO-02 - **Fiona L. Kearns**[a] Phillip Hudson[a] Stefan Boresch[b] Henry L. Woodcock[a]
[a]Department of Chemistry, University of South Florida, Tampa, FL, United States
[b]Department of Computational Biological Chemistry, University of Vienna, Vienna, Austria.

Overcoming Costly Sampling Limitations using Non-Boltzmann Bennett's Acceptance Ratio Method to Generate Potentials of Mean Force

The task of accurately conducting free energy simulations is made complicated by two discordant forces: the need for adequate sampling, and the need for accurately describing inter- and intra-molecular interactions, which is prohibitive over long simulations. In this work, the recently developed QM-NBB (Quantum Mechanical Non-Boltzmann Bennett) method has been extended to compute potentials of mean force (PMFs). Initially, a simple conformational change has been modeled – the torsional rotation around butane's central dihedral – to validate this novel free energy simulation technique. Using this new approach we were able to arrive at QM quality (e.g., HF/6-31G*) results using simulations carried out at the molecular mechanical (MM, CHARMM c36ff) and semi-empirical (SCC-DFTB) levels of theory. This new, "vertical", QM-NBB method accurately and efficiently calculates perturbations between the underlying MM and QM PMFs. This is accomplished by cleverly assembling the QM end-state ensembles from "intermediate" semi-empirical simulations and then re-evaluating simulation data at the desired Hamiltonian under the influence of a biasing potential appropriate to the differences between the two levels of theory. The data presented from this test case illustrates how well suited this new method is for overcoming costly sampling limitations when highly accurate results are desired.

CO-03 **Addison Fischer**[1], Michael Kemp[1], H. Lee Woodcock[1]
[1]Department of Chemistry, University of South Florida

Ligand-Induced Proton Transfer and Low-Barrier Hydrogen Bond Revealed by X-Ray Crystallography and QM/MM

The mechanism behind β-lactamase substrate binding has long been debated. By studying a transient low-barrier hydrogen bond (LBHB) formed between Ser70 and Lys73, the hypothesized binding mechanism for the enzyme cefotaxime-Moscow (CTX-M) can be potentially further understood. Three catalytic residues, Ser70, Lys73, and Glu166, are thought to be involved in the formation of a stabilizing transient LBHB in the active site during the attack on a β-lactam ring. LBHBs have been characterized to be shorter than normal hydrogen bonds (~2.5 Å) while being significantly stronger on the order of 5 – 10 times and are proposed to be essential in lowering the energy barrier for the enzymatic acylation of Ser70. Molecular dynamics with PROPKA3.1 will be used to determine the pKa values of the catalytic and neighboring residues. QM/MM replica path + restraint distance calculations will be calculating the proton transfer barrier energy height between

CO-04 **Ashley Parisi-Goldblatt**[1], Michael Kemp[1], H. Lee Woodcock[1]
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The Effects of Low-Barrier Hydrogen Bonds on Stability of Cefotaxime Munich (CTX-M)

Low Barrier Hydrogen Bonds (LBHBs) are 5 to 10 times stronger than the typical hydrogen bond due to shortened donor acceptor distance. Within the beta-lactamase Cefotaxime Munich (CTX-M), it is hypothesized that the LBHB between Asp246 and Asp233 could account for an increase in protein stability and will be the target of this study. An x-ray crystal structure at 0.88 Å resolution with point mutation D233N will be evaluated using molecular dynamics (MD) and quantum mechanical – molecular mechanical (QM/MM) methods. Utilizing MD and PROPKA3.1, the environment around residue 233 will be probed and compared to the native enzyme in order to elucidate the effect of the

point mutation on the local pKa values. The chemical shifts within 5A of residue 233 of the native and mutant enzymes will be analyzed via QM/MM NMR calculations to deduce the effects of LBHBs on structural elements in CTX-M.

CO-05 **Alexander Lorkowski**[1], Arjan van der Vaart[2]
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Molecular Dynamics Simulations of Corepressor-bound RXR Heterodimers

The retinoid X receptor (RXR) serves as the master partner in many nuclear receptor heterodimer complexes, which are of key importance to human disease. RXR "subordination" divides the complexes into "permissive" dimers, in which activation is achieved by binding of a RXR agonist or ligand of the binding partner, and "non-permissive" dimers, in which activation cannot be achieved by RXR ligands alone. We performed molecular dynamics simulations of corepressor (CoR) bound RARα/RXRα, PPARα/RXRα and PPARγ/RXRα complexes in the presence and absence of RXR agonists to elucidate the link between subordination and CoR release. Structural analyses showed significant differences in CoR binding between permissive and non-permissive complexes, as well as distinct responses to RXR ligand loading. The analysis is augmented with the simple confinement method (SCM) on the CoR-bound monomers, providing insights on the structural stability of the β-sheet associated with CoR-binding of RAR.

CO-06 **Md Jamilur Rahman**[1], Geoffrey Gray[1]
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Free Energy Simulations Assessing Recognition of Excise Enzymes Damaged N-7- Methylguanine

Products of non-enzymatic DNA methylation are genotoxic as it alters the expression of genes in cells during cells division or differentiation from embryonic stem cells. The recognition of excise repair enzyme for site specific m7dG is poorly understood mechanistically. CHARMM was utilized formulating the free energy simulations to analyze the DNA flexibility of the m7dG site specific. These conformational changes were conducted via step parameter analysis of free energy differences in these physical parameters-- roll and twist angles. Umbrella sampling and WHAM sampling methods were conducted for resultant graphical free energy data along the reaction coordinate of roll and twist angles. The damaged and normal DNA were compared to make the implications towards which physical step parameter influences the enzyme recognition via favorable conformation free energy changes.

CO-07 **Matthew Aubain-Santiago**[1], Adam Hogan[2], Brian Space[2]
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Modeling Sorption in MOFs with New Potential Forms

Metal-Organic Frameworks (MOFs) show promise to revolutionize a number of diverse fields which include gas storage, gas separations and catalysis. Highly accurate, transferrable, and physically based force fields are needed to properly describe and model these complex systems. Recently there has been some work in this direction. However, preliminary results suggest potential parameterization issues. Grand Canonical Monte Carlo (GCMC) simulations were performed on noble gases, CO_2, and N_2 with different MOFs, including the ZIFs and MOF-5, utilizing both Lennard-Jones (LJ) type potentials and Tang-Toennies type potentials to assess these potential issues. These MOFs are good targets because they have reliable experimental and simulation data.

CO-08 **Ariel A. Gonzalez**[1], Michael Kemp[1], H. Lee Woodcock[1]
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Density Functional Theory Benchmark Analysis of Tris(bipyridine)ruthenium(II)

In computational chemistry, Density Functional Theory (DFT) is a method for forecasting geometries and oscillator strengths of transition metal complexes employing an array of functional-basis set combinations. Articulating a combination offering a balance of accuracy and economical computational expenditure is paramount, and serves as the purpose of this work. This paper constructs a benchmark data set of geometrical parameters, and oscillator strengths for Tris(2,2′-bipyridyl)ruthenium(II). This system is widely studied for its optical properties resulting from a long-lived triplet state. Testing included 56 exchange-correlation density functionals, including local generalized gradient approximation (GGA) , hybrid GGA, meta-GGA, meta-hybrid, and long-range corrected functionals. All electron and effective-core-potential basis sets were employed. Time-dependent DFT was used to calculate vertical excitations in the system. The nuances of augmenting the scope of the basis set while calculating geometries and oscillator strengths were analyzed to find the most accurate functional-basis set combination in agreement with experimental values.

IN-01 **Janick Serrallonga**, Darrell Cole Cerrato, Christian Tang, Li-June Ming[1]
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Determining Catalytic Efficiency through Biomimetic Chemical Systems

Several aspects can determine the catalytic efficiency of an enzyme, such as active site recognition. The catalyst bio-mimicked through a metal-centered 2 – vinylpyridine and 4 – vinylpyridine were can be linked with copper as the metal in order to create the active site for the oxidation of Ditertbutylcatechol using different pyridine – copper relations (3:1, 2:1 and 1:1 pyridine to copper). In order to characterize and understand catalytic nature of the catalyst, Michaelis – Menten kinetic parameters were employed. It was found that in the presence of air (O_2), V_{max} is larger for the 3:1 pyridine:copper (21.0 nM/sec at 6mM [DTBC]) than for the 2:1 (20.0 nM/sec at 6mM [DTBC]) and 1:1 (14.0 nM/sec at 6mM [DTBC]) pyridine:copper. Future experiments will determine the relationship between various equivalences of polymer linker acrylamide to examine reactivity of more and less flexible catalysts.

IN-02 **Nicholas Varela[1]**, Kia Williams[1], Shengqian Ma[1]
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MOFs as non-PGM electrocatalyst precursors for oxygen reduction reaction

Platinum group metals are currently the conventional electrocatalysts at the cathode of polymer exchange membrane fuel cells (PEMFCs)—a promising technology in alternative energy applications. Kinetics for the oxygen reduction reaction (ORR) at the cathode are significantly slower than the H_2 oxidation at the anode. Furthermore, the high cost and limited resources of PGMs have lead to the search for efficient non-PGM electrocatalysts. MOFs have been recently explored as a new type of precursor for ORR, which exhibit superior performances compared to conventional non-PGM electrocatalysts. Here, we demonstrate the effects of metal content in self-sacrificing transition metal based MOFs.

IN-03 **Sean Jones[1]**
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The Effect of Roadway Altered Tidal Flux on Aqueous Iron (II) Concentrations in a Mangrove Ecosystem

This study examined iron (II) concentrations in pore water to indirectly determine the effects of reduced tidal flux on phosphorus concentrations versus regular tidal flux. Tidal flux is vital to the available iron present, by affecting the oxidation state in which it is found. The form of iron is directly related to the availability of aqueous phosphorus in the system. The amount of oxygen in the sediment helps to keep a balance between the various forms of iron. The site of Sawyer's Basin was selected based on the lack of plant growth and patchy mangrove distribution on the altered side of Bailey's Bluff Road in comparison to the side with regular tidal flux. A cause for these characteristics of the site could be the road obstructing the pathway of tidal water. Each pore water sample was analyzed by the colorimetric analysis of the iron (II) complex with 1,10-phenanthroline.

IN-04 **Taher Hussein[1]**, Doantrang Tran[1], Shengqian Ma[2]
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[2]Department of Chemistry, University of South Florida

Metal−Organic Frameworks as photocatalysts for carbon dioxide reduction

Utilization of Solar Energy in photocatalytic reactions for reducing carbon dioxide to fuels has caught a great deal of attention in the past decades. As the chemical reduction of CO_2 is energetically difficult due to its remarkable thermodynamic stability, this process requires a significant amount of energy transfer. Therefore, Metal−organic frameworks (MOFs), have recently emerged as a versatile platform for developing single-site solid catalysts. MOFs have been used to drive a range of reactions, including photocatalysis. MOF catalysts are easily separated from the reaction mixtures for reuse, and yet their molecular nature introduces unprecedented chemical diversity and tunability to drive a large scope of catalytic reactions. In this study, a photocatalytic reactor was designed to meet the objective of handling the reaction proposed. While designing the reactor, different parameters were considered in order to reach the optimal conversion rate. Moreover, selected MOFs were synthesized and examined for specific criteria.

IN-05 **Themelis Soulounias[1]**, Tim Vazquez[1], Shengqian Ma[1]
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Binding of metal-organic frameworks on capacitively transduced in-plane MEMS resonators for high sensitivity gas sensing

Metal-organic frameworks (MOFs) are a family crystalline materials composed of metal ions bound to organic linker molecules to form porous materials. Many of these structures contain large pore volumes and have a high affinity for small molecules, allowing for capture and storage. Resonator Micro-electro-mechanical systems (MEMS) are micro-scaled devices whose frequency is typically used as clocks for

central processing units (CPUs), but changes in their operational frequency can also be measured. By patterning MOF crystals to the MEMS device the concentrations of selected gasses in an environment can be determined with deviations in the device's operational frequency. These deviations occur in response to changes in mass when the MOFs capture gas molecules, with a theoretically limit of detection to be femtogram in mass change. The experiment studies copper and aluminum based MOFs, chosen for their air stability and affinity for methane and carbon dioxide, patterned to MEMS for gas detection.

NP-01 **Cynthia Grim**[1,2], Laurent Calcul[1,2,3], Timothy Geary[1], Vicki Muise[1], Eliane Ubalijoro[1], Bill Baker[1,2]
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[2]Center for Drug Discovery & Innovation, University of South Florida
[3]Institute of Parasitology, McGill University

Utilization of Yeast-Based Multiplex Assay to Screen Natural Products as Potential Targets for Endectocidal Drug Development

In many developing countries, neglected diseases such as parasitic infections are still a major issue of medical concern. The objective of the yeast based multiplex project is to identify new compounds that could be potential targets for developing anthelmintic medications. Saccharomyces cerevisiae strains were genetically mutated to express receptors from *Drosophila melanogaster* and *Caenorhabditis elegans* that are functionally essential for survival. These yeast strains were subjected to high through-put screening methods to test compound binding affinity to the specific neuropeptide receptors. More than 50,000 crude extracts from various fungal and bacterial sources, 3,000 fractionated compounds, and 66 pure compounds from diverse origins have been screened. Optimally, by this method we will be able to design drugs which target multiple receptor sites, thereby reducing the likelihood of parasites developing drug resistance.

NP-02 Matthew A. Knestrick[1,2] , Danielle H. Demers[1,2], Renee Fleeman[3], Lindsey N. Shaw[3], Bill J. Baker[1,2], **Bilal Arif**[1], **Jose Jesurajan**[1], **Tracy Nguyen**[1]
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[3]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida

Natural Products Drug Discovery Screening Against ESKAPE pathogens

The ESKAPE pathogens are a group of highly drug-resistant bacteria that cause well-known infectious diseases worldwide. The growing resistance to antibiotics has led to the dire need for developing new clinically relevant treatment methods. Natural products have contributed to the formation of around 2/3 drugs on the market. More specifically, the innumerable amount of endophytic fungi growing within mangrove trees provide a valuable library for obtaining secondary metabolites that may show activity against the ESKAPE pathogens. Fungi are a viable source because the harshness of their environment, in some cases, leads to natural antibiotic production. Epigenetic modifiers can help open up new biosynthetic pathways, eliciting maximum expression of the metabolites. The screening protocol includes culturing of the fungi in epigenetic modifiers, extraction and screening against the ESKAPE pathogens. Organisms that produce active compounds will be reisolated and have their active compound(s) identified. The following presentation covers samples screened to date.

NP-03 **Daniel Ramirez**[1,2]**, Steven Shaffer**[1,2], Bill Baker[1,2], Laurie Walker[3], Chad Dickey[4], Jun Tan[5]
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[4]Department of Molecular Medicine, University of South Florida
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Selected components subtractive chromatography from Camellia sinensis and other botanicals for anti-aging effects on the brain evaluation.

The leaves of the Chinese plant, Camellia sinensis, have been used as traditional medicine for thousands of years and the resulting hot evening beverage from its leaves became popular as green tea. The green tea powder, provided by the USF Botanical Gardens is a complex mixture rich in polyphenol compounds that may effect brain health. In addition to Camellia sinensis, other botanicals that may also effect brain health were boiled and subjected to subtractive chromatographic separation using preparative LC-MS at the Center of Excellence for Drug Discovery and Innovation (CDDI) Chemodiversity Facility. Fractions of selected compounds along with the corresponding remaining extracts were produced. These resulting pairs of subtracted chromatographied fractions were submitted to the College of Molecular Medicine and the Center of Excellence for Aging and Brain Repair to evaluate the bioactivity contribution and to examine the anti-inflammatory actions and prevention of reactive oxygen species production.

NP-04 **Brittany Thiessen**[1,2], **Ashley Cupaiuolo**[1,2], Elizabeth Yancey[1,2], Bill J Baker[1,2]
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[2]Center for Drug Discovery & Innovation, University of South Florida
Secondary Metabolites from Antarctic Marine Invertebrates as Sources of New Bioactivity

Isolated by the Antarctic circumpolar current, the southern oceans have unique biodiversity. They are also nutrient rich, and therefore teeming with life. Many of the organisms that life in the Antarctic waters are invertebrates, such as sponges, corals, tunicates, sea stars, and algae. These organisms produce chemistry that commonly acts as feeding deterrents or antifouling agents within their environment, but have proven to have potential medicinal value. We have begun to extract all available marine invertebrates with intention to screen these extracts for bioactivity in many different assays. Upon identification of promising bioactivity, we intend to isolate and identify the bioactive molecules via HPLC and NMR spectroscopy and mass spectrometry.

NP-05 **Nhan K. Pham[1,2],** Laurent Calcul[1,2],Bill J. Baker[1,2], Christopher Witowski[1,2]
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Isolation and Structure Elucidation of New Meridianins from Antarctic Tunicate Synoicum sp.

Marine life in Antarctica is a tremendous resource of novel compounds due to its isolated and unique habitat. A tunicate is a sessile marine organism, which relies on chemical defense to prevent predation and to adapt to the environment. The yellow top tunicate Synoicum sp. was collected off Antarctica and previously led to the report of indole alkaloids Meridianin A, B, C, and E from Dr. Baker's group. In this project, our goals are to isolate and to identify both known and potential new compounds from Synoicum sp (coll# NBP13-9). Chromatographic separation, spectroscopic and spectrometric techniques were performed during this study. All the isolated material (Meridianins A-E, and the newly found Meridianins H-J) was tested for bioactivities against *Plasmodium falciparum*, *Leishmaniasis donovani*, and *Naegleria fowleri*. All purified compounds will be added to the unique Natural Products library of the Center of Excellence for Drug Discovery and Innovation (CDDI) Chemodiversity Facility.

NP-06 **Shane Clark[1]**
[1]Department of Chemistry, University of South Florida

Anticancer potential of a marine cyanobacterium

Natural products, or secondary metabolites, are low molecular weight compounds that have been found to be beneficial to modern medicine. This is true for Symploca sp. cyanobacteria, which produces largazole, a potent anti-cancer depsipeptide currently in clinical trials. Other secondary metabolites including unique peptides produced by Symploca should be targeted for biological activity. For this purpose, a large quantity of this cyanobacterium was collected in a recent 2014 dive trip in Long Key, FL. The samples genus cannot be taxonomically identified due to morphological similarities between Symloca sp and Lynbya sp. A chemical analysis will be used to identify the exact genus and species. After exhaustive extractions, multiple purification steps including medium pressure liquid chromatography (MPLC) and high pressure liquid chromatography (HPLC) will be used to isolate compounds. Nuclear magnetic resonance (NMR) and mass spectrometry (MS) will be utilized to elucidate metabolites and bioassays will identify bioactive compounds.

NP-07 Julie Yin[1], **Nicholas Raymond[1]**
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An in Vivo and in Vitro Study of a Targeting and Activatable Supramolecule Drug Delivery System to Cancer Cells

Activatable Drug delivery with targeting modality is an active area of research and nano-scaled drug delivery systems hold tremendous potential for the treatment of neoplasms. In this study, a novel cyclodextrin (CD)-based drug delivery system for the activatable drug delivery was designed and evaluated in vivo. An adamantane-doxorubicin conjugate was synthesized with quenched fluorescence and cytotoxicity, which has been utilized as the activatable drug to be delivered by the folic acid conjugated cyclodextrin vector to folate receptor-positive [FR (+)] cancer cells. Few studies on this topic have been done as an in vitro and in vivo study with nude mice. The novel FA-conjugated β-CD based drug complex with targeting and activatable characteristics might be promising as an anti-tumor treatment for FR (+) cancer.

NP-08 **Lindsay Vacca[1,2]**, Danielle Demers[1,2], Matt Knestrick[1,2], Renee Freeman[3], Bill Baker[1,2], Lindsey Shaw[3]
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Fungal Extracts for Drug Discovery

A library of endophytic fungi isolated from tropical mangroves found throughout Florida and Mexico has been cultured, extracted, and screened against an assortment of disease causing organisms. The four main targets of interest are the ESKAPE pathogens, *Leishmania donovani*, *Naegleria fowleri*, and a variety of cancer-targets. In order to increase the probability of finding new or novel active compounds, the fungi are epigenetically modified in the culture process. Screening efforts have resulted in many active organisms. The scale-up process is a

vital step for compound elucidation and identification. Here, we will discuss the scale-up of an organism having activity against ESKAPE and *Leishmania donovani*.

NP-09 **Anna Margiotta**, **Angelina Bardell** Matthew A. Knestrick[1,2], Danielle H. Demers[1,2], Brian Vesely[3], Ala Azhari[3], Dennis E. Kyle[3], Bill J. Baker[1,2]
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[3]Department of Global Health, University of South Florida

Leishmaniasis and Natural Products Drug Discovery

Leishmaniasis, a neglected tropical disease caused by *Leishmania donovani*, is fatal untreated. The discovery of novel drugs has decreased, causing a reliance on already circulating drugs. The aim of our research is to discover new, potential compounds for drug development. Marine fungal endophytes in mangroves endure harsh conditions, producing secondary metabolites for survival. In laboratory, production of metabolites is down-regulated due to lack of stress. Epigenetic modifiers are used to activate the down-regulated biosynthetic pathways in order to access the fungi's greater chemical repertoire. The modifiers used are sodium butyrate and 5-azacytidine. Mangrove tissues from the field are plated onto growth media. Pure colonies, obtained through successive isolation, are treated with modifiers and inoculated onto rice. These are extracted with ethyl acetate, dried down, and resolvated with dimethyl sulfoxide. Extracts are screened against the parasite using an axengic amastigote and an infected macrophage model, and are tested for cytotoxicity.

NP-10 **Ariel E. Watts[1,2], Alexa Pullicin[1,2]**, Matthew Knestrick[1,2], Renee Fleeman3, Lindsay N. Shaw[3], Bill J. Baker[1,2]
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Secondary Metabolites Active Against MRSA Produced by Epigenetic Modification of a Florida Fungal Strain

Widespread antimicrobial resistance threatens the treatment and prevention of bacterial infections worldwide. The ESKAPE pathogens are a group of clinically-relevant, drug-resistant bacteria responsible for nosocomial infections. Florida mangroves are a reservoir of fungal endophytes and source of chemodiversity. Environmental pressures coax fungi to produce secondary metabolites—an invaluable compounds with antibiotic potential. Due to a marked decrease in secondary metabolite production when grown under laboratory conditions, epigenetic modification has been utilized to activate silent biosynthetic pathways, allowing for previously unreported compounds to be observed in high concentrations. A high-throughput screening project identified a fungal strain active against the ESKAPE pathogen Staphylococcus aureus. Isolated in the Tampa Bay area, the fungal strain was scaled-up and epigenetically-modified. Secondary metabolites were extracted and purified NMR was used for fractionation and purification. The fungal strain produced a derivative of a known compound observed in one of the modified-conditions and exhibited activity against methicillin-resistant S. aureus.

NP-11 **Deniz Hay[1,2],** Cynthia Grim[1,2], Andrew Schilling[1,2], Laurent Calcul[1,2], Bill Baker[1,2]
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Medium Throughput Macroorganism Extraction and Analysis

Natural products chemistry focuses on the discovery of lead compounds that are biologically active and offer therapeutic benefits. Nearly 50% of all new drug entities between 2000 and 2010 are from biological sources or are derivatives of natural products. To speed up the rate at which compounds can be screened there are two methods to do so, combinatorial and crude. For this study crude extracts will be used to screen against *Naegleria Fowleri*. Macroorganisms of interests will be extracted using polar and nonpolar solvent system extractions (SSE). Macroorganisms that show positive activity will then be partitioned and further screened to determine exact active compounds. The ecological diversity of marine macroorganisms being screened in the assay will open new doors to promising species with disease eliminating secondary metabolites.

NP-12 **Riley Bednar[1], Ilya Luschitsky[1]**, Christopher Witowski[1,2], Bill Baker[1,2]
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Re-isolation of Co-culture Induced Bipolarolides from a Marine-Derived Bipolaris sp. Fungus

The bipolarolides are a new class of polyketide natural products isolated from a sponge-derived fungus. These compounds were shown to be upregulated in competition with Aspergillus niger, a common fungal contaminant, including bipolarolide C which was produced de novo in co-cultures. The limited amount of material (0.008% yield from extracts) hindered attempts at crystallization for stereochemical determination and screening for antimicrobial bioactivity. Previous optimization extracts from the two fungi were combined to re-isolate more of these

precious secondary metabolites. Purification was done using high-pressure liquid chromatography (HPLC) and dereplication with high-resolution mass spectrometry (MS) and nuclear magnetic resonance (NMR) was used to identify these compounds during fractionation.

OR-01 **Kaitlyn Hite**[1], Jess Jones[1]

[1]School of Arts and Sciences, Saint Leo University

Ultrasonic conditions improves SNAr reaction between 1-halo-4-nitrobenzenes and imidazole.

Ultrasonic conditions improves SNAr reaction between 1-halo-4-nitrobenzenes and imidazole. K.HITE and J.JONES. Sonochemistry, a widely researched sector of green chemistry, can be used as an alternative method in synthesizing many common organic substances. In using ultrasound, less energy is consumed, less hazardous waste products are created, and less toxic chemicals are needed to drive reactions as compared to reactions run under traditional thermal conditions. Ultrasound has proven successful previously in driving the inorganic base-catalyzed reaction of imidazole with 1-halo-4-nitrobenzenes to form 1-(4-nitrophenyl)-imidazole under a nucleophilic aromatic substitution mechanism (SNAr). Using an ultrasonic cleaning bath (40 kHz, 110 W) in place of the traditional probe sonicator system, the SNAr reaction was optimized via the variation of leaving groups, inorganic bases used, and the ratio of imidazole and base to the halobenzene. It was observed that a larger nucleophile to halobenzene ratio and a 1.62:1 halonitrobenzene to potassium carbonate ratio were optimal.

OR-02 **Carrie Robart**[1], Ali Husain[1], Arthur Maknenko[1], Kirpal Bisht[1]
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Synthesis of N-Carboxy-Cyclic Anhydrides

The synthesis of polypeptides by ring-opening polymerization is an attractive approach to their synthesis for material science applications. The purpose of this study is to convert commercially available amino acids to the N-carboxy-cyclic anhydride (NCA) monomers. The synthesis of the NCAs was attempted in a two-step procedure-(1) by forming the benzyloxycarbonyl or the tert-Butoxycarbonyl amino acids and then (2) cyclization to produce the NCAs. The results of the investigation will be presented.

OR-03 **Tyler Wickas**[1], Faeez Mahzamani[1], Renee Fleeman[2], Lindsey Shaw[2], Edward Turos[1]
[1]Department of Chemistry, University of South Florida
[2]Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida

Synthesis and Antibacterial Activities of Chiral N-Acyl Ciprofloxacins Against ESKAPE Pathogens

Our laboratory has been synthesizing and evaluating synthetic antibacterial agents for use against deadly ESKAPE bacteria, which are highly resistant to most current antibiotics. Our studies are focusing on new N-acylated ciprofloxacin in which the N-acyl moiety is chiral. These compounds are being prepared by N-acylation of ciprofloxacin, a commercial antibiotic used to treat various bacterial pathogens. Our presentation will discuss the results we have obtained in terms of the chemical structures and antibacterial activities of these new derivatives against ESKAPE pathogens.

OR-04 **Saskia Sassine**[1], **David Desena**[1], **Michael Inman**[1]
[1]Department of Chemistry, University of South Florida

Peptide- Peptoid Library

Previous work in our lab has successfully developed a peptide-peptoid hybrid scaffold that is based off of a cyclic B-hairpin turn. In the future this scaffold will be used to create a combinatorial library for screening hits to varying targets. The peptoid component of the hybrid compound is advantageous to the overall library diversity due the fact that there are an estimated 500-1000 times more primary amines than amino acids commercially available. Our main objective in this project was to develop new primary amines for incorporation into the scaffold. Several organic synthetic schemes were utilized to identify the best method for the creation of these amines. Efforts were directed toward a successful route that minimized time and materials. Chromatographic and spectroscopic techniques proved that this efficient route resulted in high yields of pure primary amines scalable to 10 grams of product.

OR-05 **Amber Hodge**[1], Yan Shi[1], Jianfeng Cai[1]
[1]Department of Chemistry, University of South Florida

The building blocks of the AA-peptide

Amino acids are the basic building blocks of peptide chains. The building blocks of AA-peptides are synthesized as a secondary amine that is acylated with various carboxylic acids from the reaction of amino acid esters with Fmoc-amino ethyl aldehyde. The AA-peptides are a class of mimic peptides that resemble natural α-peptides. These peptide mimics are oligomers of N-acylated-N-aminoethyl amino acids. The newly synthesized γ-AApeptide has a modified framework of the AA-peptide in that it is composed of γ-substituted-N-acylated-N-amino-ethyl amino acids. There are copious biomedical applications that arise with the use of this peptide mimic. It is resistant to hydrolysis and proteolysis, which makes the synthesis and utilization of the peptide effortless. This peptide mimic is used to influence protein-protein interaction as well as cell signaling processes. These results can be applied to future drug therapies in malignancies such as cancer, neurodegenerative diseases, and human immunodeficiency viruses.

OR-06 **Mario Fiumara**[1], Weiji Zhang[1,2]
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[2]Jiangnan University, China

Synthesis of 5,15-Bis (3,5-Diisobutoxycarbonylbiphenyl) Porphyrin

Through the use of a step wise synthesis the aim is to generate a more efficient way to produce 5,15-Bis (3,5-Diisobutoxycarbonylbiphenyl) Porphyrin. The current method for the generation works but there is still room for improvement. This volume of improvement that is available is what this experiment is aiming to reduce, either by generating a higher percent yield of equal purity or the same yield with a higher purity. To prove the yield the product produced is being tested with numerous tests including (but not limited to) UV/Visible light spectroscopy, and NMR, and will be compared to the factory produced standard as a control.

OR-07 **Nicholas Wallace**[1]
[1]Department of Chemistry, University of South Florida

Forming Possible Drug Candidates for Leishmaniasis through Organic Synthesis

Leishmaniasis is a disease caused by the parasites of the genus Leishmania, affecting more than two million new people and accounting for anywhere between twenty and fifty thousand deaths every year. It is contracted through the bite of sandflies, which commonly occur in the less developed countries. A form of the chaperone heat shock protein (Hsp) 90 plays a critical role in the life cycle of *Leishmania donovani*, so finding compounds that can selectively inhibit this protein can subsequently hinder the disease by interfering with the growth of the parasite. Through the use of organic synthesis, we have identified a novel scaffold that includes compounds that inhibit the growth of *L. donovani*.

OR-08 **Aaron Parise**[1], Demetrios Pantages[1], Si Yi[1], Jon C. Antilla[1]
[1]Department of Chemistry, University of South Florida

Phosphoric Acid Mediated Catalytic Enantioselective One-Pot Amination of Oxindoles With Substituted Benzylimines.

Although enantioselective reactions for the synthesis of 3, 3-di-subsituted oxindoles are known in the literature, methods which use a Chiral Phosphoric Acid (CPA) catalyst are rare. Development of a methodology for the synthesis of 3, 3-di-subsituted oxindoles in an efficient and inexpensive one-pot fashion would be of interest to synthetic chemists. The preliminary results reported herein show a facile route to 3, 3-di-substituted aryloxindoles via an enantioselective CPA catalyzed reaction of 3-substituted 3-aryloxindoles with imines using 3, 3'-α-napthal phosphoric acid as the catalyst.

OR-09 **Charles K. Harvey IV**[1], C. Eric Ballard[1]
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Titanium(IV) Isopropoxide-Promoted Hydrosilylation of Unsaturated Functional Groups

Exposure of diarylacetylenes to titanium(IV) isopropoxide and triethylsilane followed by aqueous workup resulted in reduced products. The scope of this transformation with respect to alkene and alkyne substrate and compatibility with other functional groups, particularly carbonyl units. Results of initial mechanistic studies will also be reported.

OR-10 **Ali Siddiqui**[1], Zachary Shultz[1], James Leahy[1]
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Progress towards an enantioselective synthesis of membranolide A

Sea sponges are responsible for the production of a broad range of secondary metabolites, many of which possess bioactivity. Specifically, Dendrilla membranosa is an Antarctic sea sponge that has been found to produce a family of compounds known as the membranolides. There are four recognized membranolides: membranolide A, membranolide B, membranolide C, and membranolide D. Membranolide A has been shown to possess antimicrobial bioactivity against Staphylococcus aureus. Furthermore, the relative stereochemistry of membranolide A is known, however the absolute stereochemistry is currently unknown. Establishment of the absolute stereochemistry of membranolide A may prove valuable to future exploration of the antimicrobial applications of this compound. Thus, this study seeks to elucidate the absolute stereochemistry of membranolide A via total synthesis.

OR-11 **Matthew Jacobsen**[1], Ali Husain[1], Kirpal Bisht[1]
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Synthesis of Water Soluble Recorcin[4]arene Decorated with Glucose/Maltose Monomers via Cu(II) Catalyzed Cycloaddition (CuAAC)

Environmentally friendly chemical synthesis is a major concern in organic synthesis. By eliminating the use of organic solvents as a media in chemical reactions, a number of green chemistry processes can be employed. Water has many advantages over organic solvents which are toxic, flammable, volatile and expensive. Water in general is cheap, reusable, and environmentally friendly. Through click chemistry, Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC), novel resorcin[4]arene cavitands were designed and synthesized by modifying them with β-glucose and β-maltose monomers via multi-1,4-distributed 1,2,3-triazoles. The novel cavitands were synthesized by enforcing the glycocluster moieties to cover the resorcin[4]arene hydrophibic cavity, enforcing solubility in an aqueous media. Additionally, the remarkable structure of resorcin[4]arene cavitand consisting of four resorcinol monomers provides a cavity which can accommodate other guest molecules. Their ability to solubilize in an aqueous environment can be employed to do different organic transformations as a catalyst.

OR-12 **Vincent Bedami,**[*1] **Sridhar R. Kaulagari,**[6] Rajesh R. Nair,1,6 Priyesh Jain, 1,6 Yi Liang,1 Michael F. Emmons,4 Anthony W. Gebhard,3 Lori A. Hazlehurst, 2,3,5,6 and Mark L. McLaughlin.[1,3,4,6]
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Cyclic β-Hairpin-like Peptidomimetic MTI-101 Inhibit Cell Adhesion in Multiple Myeloma

Multiple Myeloma (MM) remains as an incurable malignancy in spite of recent advances in understanding of the disease. HYD1 is an integrin antagonist that lacks the RGD motif and reverses resistance to standard therapy and induces programmed cell necrosis as a single agent in vitro and in vivo. The display of core residues of HYD1 in the strand portion of a cyclic beta-hairpin-like scaffold increases its bioactivity which led us to MTI-101 as a lead drug candidate. Herein, we report work on improving the half-life and efficacy of our lead.

OR-13 **James McDaniel**[1], Grant Simpson[1], Khanh Ha[1], Charles Hall[1], Alan Katritzky[1]
[1]Department of Chemistry, University of Florida

Hydroxyproline Ligation in Coupling of Peptide Fragments

The development of chemoselective ligation represents a major interest in synthetic peptide chemistry. The first major breakthrough in this approach began with the discovery of native chemical ligation. During the last two decades, major research efforts have been focused on applying this approach to other amino acid sites of ligation. Proline reacts at the slowest rate of all natural amino acids in native chemical ligation, due to non-covalent electronic effects of the unique orientation of amide carbonyls in Xaa-Pro peptidic linkages. To address this problem of proline-site ligation, we developed a hydroxyproline ligation strategy, based on native chemical ligation “capture-rearrangement” principles, utilizing hydroxylproline's chemoselective bifunctionality. We successfully demonstrated that this approach achieves ligation at difficult proline sites in a generalizable fashion. Additionally, we studied the mechanism of hydroxyproline-site ligation to further understand this reaction. We successfully isolated the key bridged bicyclic aminal intermediate which verifies the proposed mechanism.

OR-14 **Nicholas Clough**[1]
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Enantioselective Aza-Friedel-Crafts Reaction of Phenols with Imines by Chiral Phosphoric Acids

Presently, the Friedel-Crafts reaction is a useful tool for the formation of carbon-carbon bonds. In the past twenty years, the employment of chiral organocatalysts in such reactions has shown enantioselectivity and high yield for the desired products. As chiral amines are prevalent in medically important compounds, a convenient synthesis is valuable and possible by asymmetric aza-Friedel-Crafts reactions. Chiral phosphoric acids (CPA) are known to promote enantioselectivity in the Friedel-Crafts reaction of indoles with imines and the aza-Friedel-Crafts reaction of indoles with lactams. For this work the viability of CPAs as organocatalysts in the aza-Friedel-Crafts reaction of phenols with imines will be examined. Analysis of the synthesized substrates and final products will be done by 1H NMR, IR, MS. Enantiomeric excess will be determined using HPLC.

OR-15 **Joshua McBride**[1], Susana Lopez[1], Jon Antilla[1]
[1]Department of Chemistry, University of South Florida

A quick and reliable synthesis for α,β-unsaturated Weinreb amides

α,β-unsaturated Weinreb amides (WA)serve as diverse synthons in organic chemistry. Although, known methods for the preparation of WA exist, a shorter and more direct route to the product would prove advantageous. Currently, the most utilized method involves a Honer-Wadsworth-Emmons olefination to the ethyl ester, which can then be readily converted to the WA. Herein is reported a method by which the WA can be accessed in one-step from various commercially available ketones or aldehydes. Starting with a simple procedure for the preparation of a specialized ylide, a wide variety of WA can be synthesized in high yields and good stereoselectivity.

OR-16 **Nicholas Kalogeras**[1], Hasnaa Mouttaki[1], Edward Turos[1], Keriann Greenhalgh[2]
[1]Department of Chemistry, University of South Florida
[2]KeriCure Inc.

Polymerizing Acrylates to Develop Healthcare Products to Release to Market

Working with KeriCure Inc., the objective of this research is to develop a new health product and release it into the public market. The main objective is to take the current liquid seal product and allow it to reach a new antibacterial level rather than just a protective and preventative sealant. An additional string of research is also being conducted to create a more pleasant aroma from the polymer itself. The goal is to insert perfuming products into this product as well. This research looks to create a liquid bandage product and have this product assist the immune system in antibacterial activity in the body. This body of research deals with polymerizing various acrylates to create a polyacrylate polymer that is all natural and out performs all other liquid bandages on the market through its additional effects.

OR-17 **Christopher S. Sebastiano**[1], Rachel A. Jones[1], C. Dennis Hall[1]
[1]Department of Chemistry, University of Florida

Synthesis and Fluorescent Studies of Amino-Coumarin Conjugates as Biological Probes

Coumarins are naturally occurring phenolic compounds of which 2H-1-benzo-pyran-2-one (coumarin) is the parent compound. They can be easily synthesized either via the Pechmann or Knoevenagel condensation, which has facilitated the study of this class of compound. Both synthetic and naturally occurring coumarins have shown a wide range of pharmaceutical activities, including anti-coagulant, anti-cancer, antioxidant or antiviral properties. The activity of each coumarin is dependent upon both the choice of functionalization and the substitution pattern in the heterocyclic scaffold. The labeling of peptides with fluorescent tags provides a powerful tool for the investigation of biological processes including the in vivo analysis of cell function, detecting enzymes and the study of signaling recognition events. The fluorescent properties of coumarins have led to their use as highly sensitive biological probes with applications including thiol detection, protein function and cell structure studies. We report herein the synthesis and fluorescent properties of Amino-Coumarin Conjugates.

OR-18 **Sri Harsha Palakurty**[1]
[1]Department of Chemistry, University of South Florida

Synthesis of dihydroindazole compound

One of the strategies is the synthesis of 1-cyclopropylidenepropan-2-one, through the use of 1-(triphenylphosphoranylidene)propan-2-one and (1-ethoxycyclopropoxy)trimethylsilane. This has shown to be a difficult process with adversities around every corner, from the creation of the product to the purification of it. We are trying a new method of synthesizing this in a cluster of solvents in order to find out the best method for the desired synthesis. Another part of the project is the synthesis of 7-fluoroquinazolin-4-amine. We are currently in the process of purifying the material so that we can see the quantity of the molecule that is present in the solution. We expect the reaction to have proceeded and for good yields to be obtained.

OR-19 James W. Leahy[1], **Anika Graham**[2], **Margarita Vanegas**[1], **Elizabeth Shald**[1]
[1]University of South Florida
[2]Center for Drug Discovery & Innovation, University of South Florida

Synthesis of xanthurenic acid analogues as tools for the discovery of novel antimalarial agents

Infectious diseases are the second leading cause of all human death worldwide. In 2010, there were ~200 million cases and 660,000 deaths due to malaria. The parasitic source of transmission is Apicomplexa of the genus Plasmodium. Human infection occurs through sporozoites, which move into the liver to mature into merozoites and infect red blood cells. Gametogenesis does not proceed until these cells are ingested by a mosquito to form new sporozoites and restart the cycle. The purpose of this project is to retard the ability of gametocytes to enter the mosquito vector by forcing their premature differentiation and keeping them as merozoites inside the host. Xanthurenic acid is the activating chemical factor responsible for initiating gametogenesis in the mosquito's gut. Therefore in this project, we are synthesizing analogs that will retain the ability to coordinate with metal ions while introducing a site for the appendage of vital functionality for derivatization.

OR-20 **Angel Gomez**[1], Garrett Craft
[1]Department of Chemistry, University of South Florida

Drug Delivery via Biocompatible Composites

Methacrylate hydrogels synthesized with copper paddlewheel filler material will be assayed for applications in controlled drug release. Hydrogels are polymeric materials which can absorb large amounts of water, and coupled with their porosity make them quite similar to human tissue. The filler material along with HEMA will serve to crosslink the polymer chains and is proposed to modulate the diffusive properties of the material. The paddlewheels contain two coppers that coordinate with four carboxylate ligands at near 90 degree angles. The paddlewheel material can form hydrogen bonds via their ligand's hydroxyl groups, serving as crosslinkers between the methacrylate pendant groups of the polymer. The aim of this project is to ultimately provide a biocompatible material that intrinsically delivers drugs over prolonged periods of time. Differential Scanning Calorimetry, UV-Vis and FT-IR spectrophotometery are techniques used to characterize these hydrogel materials and their diffusive properties.

OR-21 Andrea Lemus[1], **Kevin Petersen**[1], James Leahy[1]
[1]Department of Chemistry, University of South Florida

Novel Synthesis of (+)-Catechin Metabolites

Catechin is a secondary metabolite that is present in most plants. When digested by animals, catechin is broken down into smaller molecules by the liver and intestines. This class of molecules has anti-inflammatory properties and may be useful in diabetes research. The goal of our research is to synthesize two catechin metabolites so they can be externally evaluated to determine how they may be useful for diabetes pathways. The two target compounds 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. Preliminary testing of these synthesized compounds indicates that they have mild anti-inflammatory properties. Further research on these compounds involves making enantiomerically pure compounds for greater accuracy in the biological assays, in hopes that one will be more biologically effective than another.

OR-22 **Catherine Costa**[1], James Leahy[1], Benjamin Eduful[1], Brian Vesely[1], Ala Azhari[2], Dennis Kyle[2]
[1]Department of Chemistry, University of South Florida
[2]Department of Global Health, University of South Florida

Synthesis of Anthranilamide Derivatives of Hsp90 Inhibitors as Anitleishmaniasis Agents

Leishmaniasis is a disease caused by parasitic protozoa; it is spread through the bite of a sand fly carrying the infection. This presentation reports on the search for molecules that prevent this illness presumably through the inhibition of the protozoan ortholog of the molecular chaperone heat shock protein 90. Hsp90 is a protein that controls both the heat shock response and the morphological differentiation that has been implicated in several therapeutic areas. A screening campaign revealed a potential lead compound that has been verified and anthranilamide analogs have been synthesized. Currently more derivatives are under investigation with the goal that an active hsp90 inhibitor, that has suitable pharmacological properties, will be produced. This molecule can then be used as a potential treatment for leishmaniasis.

OR-23 **Sierra Teegarden[1]**, Ahnaf Siddique[1], Justin Jimmy[1], Hyun Joo Kil[1], Michael Doligalski[1], Mark Mclaughlin[1]
[1]Department of Chemistry, University of South Florida

Synthesizing Amines for Stapled Peptoid-Peptide Hybrids

Peptoids, which mimic regular peptides but have side chains attached to the nitrogen atom on the peptide backbone rather than to the alpha carbon, have much more diversity. However, peptoids cannot naturally self-assemble into the beta-hairpin preferred secondary structure because they lack backbone hydrogen bonding capabilities of a normal peptide. To allow for both structural diversity and secondary structure a large scale of highly pure primary amines were synthesized, which are fundamental units for peptoid-peptide hybrids.

OR-24 **Josue Liriano[1]**, Susana S. Lopez[1], Jon Antilla[1]
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Chiral phosphoric acid-catalyzed Friedel-Crafts Alkylation of indoles at the 2-position

Indoles are of great interest to synthetic organic chemists due to the significant number of biologically active natural products, which contain this scaffold. From the medicinal chemistry perspective, these privileged structures represent an important component in many approved pharmaceuticals used as therapeutic agents. Substituted indoles, especially those substituted at the 2-position, are latent intermediates for numerous alkaloids and pharmacologically important substances. Alkylation methods using the well-known Friedel-Crafts reaction have been of significant interest in recent years. Developing enantioselective methodologies which can perform these transformations using organocatalysts can expand the already important synthetic utility of indoles. The work presented herein describes the development of a methodology for an enantioselective Friedel-Crafts alkylation reaction of indoles at the 2-position by a BINOL-derived phosphoric acid.

OR-25 **Giovanni Rodríguez[1]**, Johanna Fajardo[1], Yanira Enríquez[1], Ingrid Montes[1] Ana Guadalupe[1]
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Synthesis of Novel Ferrocene Chalcones Derivative's Polymers

Since the discovery of ferrocene in 1951, it has been used to synthesize derivatives that exhibit a variety of applications, including: biocatalysis, biosensing, materials sciences, biofuel cells, films, anticancer agents, biomedical engineering, electroactive materials, aerospace materials, surface science, biophysics, and biological activity. Ferrocene derivatives show different electronic, optical, and redox properties due to their structure and among the possible applications, they can be used to prepare a series of electrochemical labels for the detection of DNA hybridization. The main goal of this research is to synthesize and characterize new ferrocene polymers from ferrocenyl chalcones and explore their potential applications. The general objective is accomplished by the synthesis of a series of ferrocenyl chalcone derivatives that encompasses a Claisen-Schmidt condensation to obtain the nitro ferrocenyl chalcones, then a chemioselective reduction of the nitro group, followed by the amidation of a phenylamine substrate to synthesize the monomers as the precursors for co- and terpolymers after applying a free radical reaction. Ferrocenyl chalcone derivatives and ferrocene polymers were obtained in good to moderate yields that vary from 64% to 86%. The characterization of these polymers has been achieved using, IR spectroscopy, UV-Vis, and electrochemistry. The synthetic methodology and characterization of these compounds will be elaborated.

OR-26 **Noreen M. Haq[1]**, Michael L. Doligalski[1,2], Amanda S. Huynh[1,2], Josef Vagner[3], David L. Morse[1], Mark L. McLaughlin[1]
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[2]H. Lee Moffitt Cancer Center, Tampa, Florida
[3]BIO5 Institute, Tucson, Arizona

Synthesis of New Toll-Like Receptors 2 (TLR2) Ligands for Pancreatic Cancer Imaging

A cornerstone of pancreatic cancer treatment is surgical resection, without which, the 5-year survival rate is 6% vs. 20 – 25%. Toll-like Receptor 2's (TLR2) are a type I transmembrane glycoprotein that are overexpressed on pancreatic tumor cells, making them useful in monitoring the removal of cancers in the operating suite. This project was designed to elucidate a peptidomimetic ligand for pancreatic TLR2 in order to incorporate a fluorescent molecular tag meant to improve the imaging of cancerous cells. The project involved, first, optimizing the synthetic strategy for the monoacylated PAM monomer of the ligand. Next, the monomer was incorporated into the polypeptide using Nα-Fmoc solid phase peptide synthesis technique. Finally, a fluorescent dye conjugate was prepared and attached to the N-terminus of the ligand. The ligand was prepared with high yield and purity levels. Future work will characterize the importance of this fluorescent ligand in the imaging of pancreatic cancer.

OR-27 **Ansley Howard,** Yassin El Batrawi, Javier Cuevas, John Antilla
Department of Chemistry, University of South Florida

The Investigation of Ca^{2+} deregulation in the Treatment of Non-Small Cell Lung Cancer (NSCLC)

Farnesyltransferase inhibitors (FTIs) such as tipifarnib have shown anti-proliferative activity against non-small cell lung cancer (NSCLC). It is hypothesized that the FTase inhibitory effect alone is insufficient for anti-cancer activity and that the disruption of Ca^{2+} homeostasis within the tumor cells via interaction with the over-expressed Orai3 constituent of the store-operated channel (SOC) is necessary. A benzofuran analogue of tipifarnib previously synthesized by Asoh et al. showing high FTase inhibitory activity but low anti-proliferative effect is being used to test this hypothesis.

OR-28 **Teh, Wei Pin**; Bromfield Lee, Deborah
Florida Southern College

Studies towards the synthesis of Stachybotrin D.

Recently, 7 novel phenylspirodrimanes were isolated from Stachybotrys Chartarum MXH-X73 by a group from China while in search of bioactive secondary metabolites. Stachybotrin D, has shown inhibitory effects on the reverse transcriptase of HIV. The phenylspirodrimanes are a class of molecules mainly isolated from Stachybotrys species, which its structure contains three main classes: tetracyclic aromatic sesquiterpenoids, pentacyclic aromatic sesquiterpenoids and the stachyflins with a pentacyclic moiety including a cis-fused decalin. These compounds have shown diverse bioactivities, from targeting tyrosine kinase, cholesterol esterase to HIV-1 protease and endothelin, thus making them a class of compounds that are interesting and potentially useful in pharmacology. Overall, with developing a synthetic methodology for the phenylspirodrimanes, we will be able to design and synthesize various derivatives of these compounds that could potentially be promising class of drugs. Our key step in this synthesis is the formation of spirobenzofuran, utilizing an asymmetric Grignard reaction and follow by a condensation reaction.