12th Raymond N. Castle Student Research Conference

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Welcome from the Castle Conference Committee

Dear Colleagues and Friends,

Welcome to the 12th 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. George Christou. 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. Christou will be giving a presentation on one aspect of his exciting research, entitled *Manganese-Oxo Chemistry: From Molecules as Nanoscale Magnets to Nature's Choice for the Photosynthetic Oxygen-Evolving Complex.*

Lastly, we would like to thank all that chose to volunteer their time and efforts, particularly the judges; our financial advisors Debbie Gee, Kim Read, Brenda Simmons; our incomparable office staff Roberto Avergonzado, Cheryl Graham and Linda Lowe; and especially Dr. Laura Anderson for helping us plan and coordinate this year's conference. We would also like to acknowledge the other faculty who were instrumental in this year's conference: Dr. Kimberly Fields, Dr. Vicky Lykourinou, Dr. Patricia Muisener, Dr. Santiago Sandi-Urena, and Dr. Edward Turos. In addition, we are grateful for the financial support that allows us to host this conference and owe special thanks to Agilent, Shimadzu, 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 12th Raymond N. Castle Student Research Conference.

Sincerely,

The Castle Conference Committee

12th Raymond N. Castle Conference Committee

Committee Members:
Joseph Gill (Chair)
Jennifer Borja
Cole Cerrato
Chris Cioce
Danielle Demers
Wenyang Gao
Jacqueline Fries
Parker Hutha
Yujuan Liu
Hasnaa Moutakki
Sri Nimmagadda
Christie Tang
Justin White
Elizabeth Yancy

Faculty Advisor:
Dr. Laura Anderson

Supporting Faculty:
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Dr. Julio Garay
Dr. Vicky Lykourinou
Dr. Li-june Ming
Dr. Patricia Muisener
Dr. Santiago Sandi-Urena
Dr. Edward Turos

Web Support:
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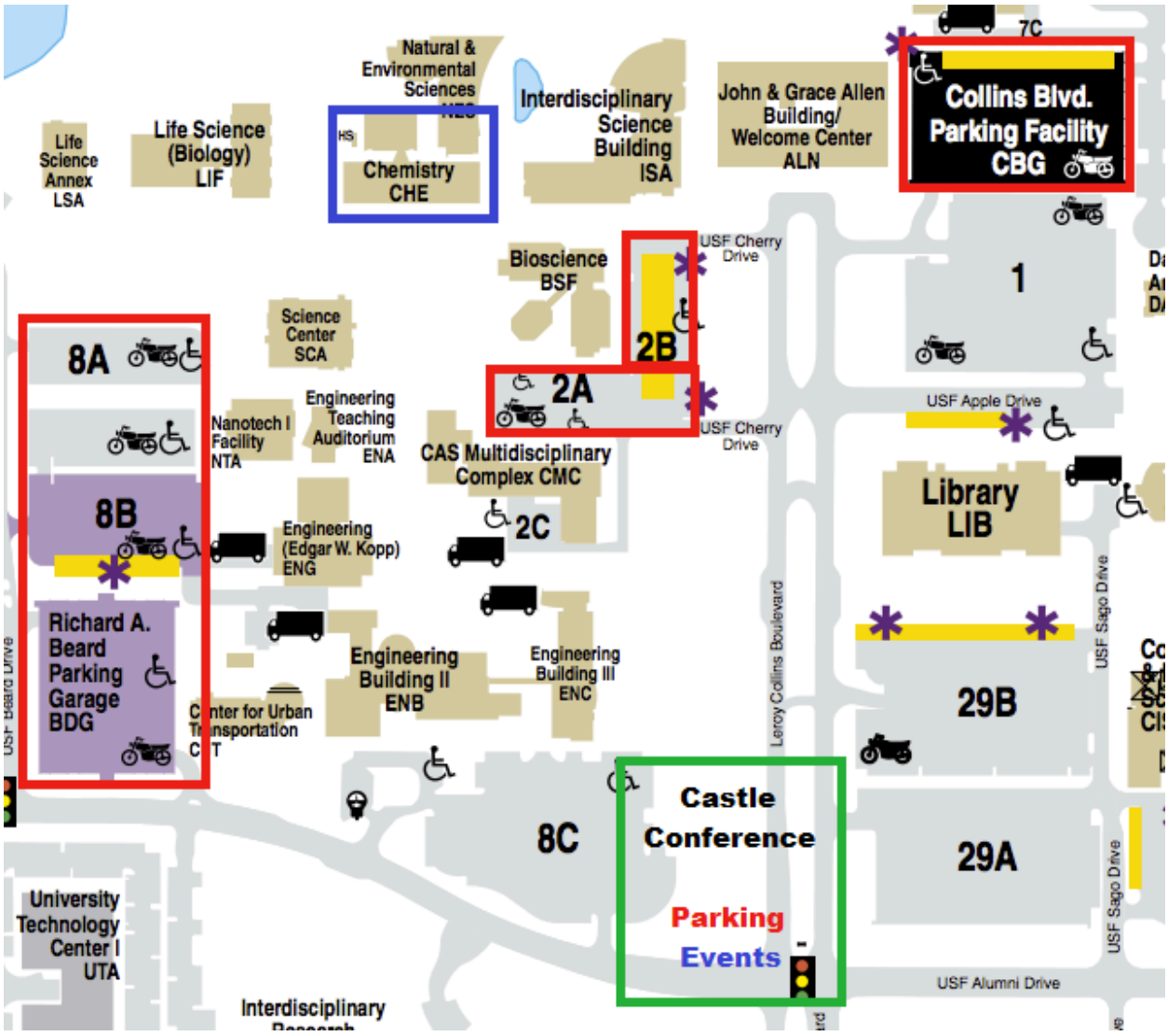
Building Map



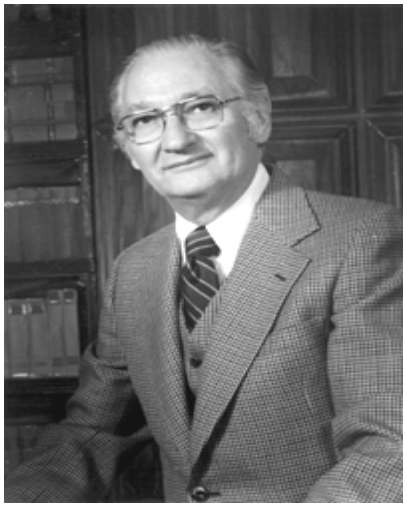
Schedule of Events

Saturday, April 12, 2014

7:45 AM	-	8:30 AM	**Welcome Session** - *Registration and Breakfast*	Chemistry Courtyard
8:30 AM	-	10:00 AM	**Morning Talk Sessions I & II** *Graduate Student Presentations*	CHE 100 & CHE 111
10:00 AM	-	10:15 AM	**Break**	
10:15 AM	-	10:35 AM	**Castle Conference Introduction** *Professor Edward Turos*	CHE 100
10:35 AM	-	11:15 AM	**New Faculty Presentations** *Professors Jeffrey Raker, Scott Lewis, Yiannis Gelis*	CHE 100
11:20 AM	-	12:20 PM	**Plenary Speaker - Professor George Christou** *Manganese-Oxo Chemistry: From Molecules as Nanoscale Magnets to Nature's Choice for the Photosynthetic Oxygen-Evolving Complex*	CHE 100
12:20 PM	-	1:30 PM	**Lunch** *Sponsored by Tampa Bay Local American Chemical Society*	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	-	5:00 PM	**Afternoon Talk Sessions I & II** *Graduate Student Presentations*	CHE 100 & CHE 111
5:00 PM	-	5:15 PM	**Break**	
5:15 PM	-	5:30 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.

Professor George Christou

Plenary Speaker

George Christou was born on the Mediterranean island of Cyprus, but grew up in London, England. He obtained his BSc and Ph.D. degrees at Exeter University. His Ph.D. was in Organic Chemistry, working with H. N. Rydon, and involved the synthesis by classical methods of cysteine-glycine polypeptides and their use as ligands to iron-sulfur clusters to model the ferredoxin proteins. After a NATO Postdoctoral Fellowship with R. H. Holm at Stanford and Harvard Universities in bioinorganic chemistry targeted at the Mo/Fe/S cluster of the nitrogenase enzyme, he took up his first faculty position at Imperial College, London, in 1982, and initiated his interest in manganese chemistry that continues to this day. Two years later he moved to Indiana University, Bloomington, where he rose through the ranks to Blough Professor. In 2001, he moved to the University of Florida to take up his present position as the inaugural holder of the Drago Chair of Chemistry and was subsequently also promoted to Distinguished Professor.

Professor Christou's research interests are in transition metal chemistry. He is particularly interested in 3d metal-oxo cluster chemistry and its applications to fields such as bioinorganic chemistry, supramolecular chemistry and nanoscale magnetic materials. In the latter area, he has been a leading figure in the development of the magnetic phenomenon of single-molecule magnetism, the ability of individual molecules to function as nanoscale magnets. These have potential applications in ultra-high-density information storage, quantum computing, spintronics, and other specialized areas. In bioinorganic chemistry, he has long been fascinated by the Mn4Ca cluster that carries out water oxidation to oxygen gas during photosynthesis in plants and cyanobacteria, the origin of almost all the oxygen gas on this planet. In more recent years, he has worked in a variety of other areas, such as supramolecular chemistry applied to magnetic molecules, molecular crystals of wheel-like clusters as porous materials, and the use of Mn and Mn/Ce clusters as catalysts. He has collaborated over the years with many types of spectroscopists and physicists, including quantum physicists who have probed the fascinating quantum properties of his single-molecule magnets and other magnetic molecules. His work has led to 544 publications (as of March 1, 2014), of which 67 papers are in the physics literature.

Dr. Christou has received a large number of prestigious awards and honors over the years, including an Alfred P. Sloan Foundation Fellowship, a Camille and Henry Dreyfus Foundation Teacher-Scholar Award, the 1986 Corday-Morgan Medal of the UK Royal Society of Chemistry, the 1993 Dwyer Medal of the Australian Chemical Society, the 2000 Award for Chemistry and Electrochemistry of Transition Metals from the RSC, the 2008 Florida Award of the ACS Southeastern region, among others. He is an Honorary Professor of the London Centre for Nanotechnology and University College, London.

Professor Christou is very active in state and international conference organization. He founded the Florida Inorganic and Materials Symposium (FIMS) student meeting held in Gainesville every year, which

has grown in popularity and now encompasses 14 Florida universities and colleges. He also co-founded and co-organizes every year two alternating biennial workshops, the specialized Current Trends in Molecular and Nanoscale Magnetism (CTMNM) workshops spanning chemistry and physics in even years, and the broad North America-Greece-Cyprus Workshop on Paramagnetic Materials (NAGC) spanning chemistry, physics, biochemistry, medicine, and materials science in odd years. These workshops strongly emphasize broad programs and inclusion of many talks from junior people (students and postdocs).

Professor Dean F. 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 Barbara 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. Dr. 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. Dr. and Barbara Martin were the co-recipients of the 1994 Medalist Award of the Florida Academy of Sciences, its highest award. Professor Martin has been active in the Florida Section of the American Chemical Society (Chairman, 1986), and 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.

Dr. Solomon T. Weldegirma

Special Thanks

Dr. Solomon T. Weldegirma received his B.S., with Honors, from Asmara University, Eritrea in 1989. He focused his graduate studies on extraction of active compounds from natural products through organic chemistry, earning his M.S. in 1995 from Addis Ababa University, Ethiopia. During this time, he worked in the Food Industry heading up Research, Quality Control, and Development Departments, with companies that shared his passion for the importance of natural products. Under the guidance of Professors Frode Rise and Lise-Lotte Gundersen, Dr. Weldegirma received his Ph.D. in Synthetic Organic Chemistry from the University of Oslo, Norway, in 2004, where he studied indolizine compounds as possible inhibitors for a variety of targets. In 2005, he took a Post- doctoral fellowship under Dr. Bill Baker at the University of South Florida, studying degradation of natural products.

Since 2006, Dr. Weldegirma has shared his love of organic chemistry with students at the University of South Florida as the Organic Chemistry Laboratory Coordinator and Instructor of Organic Chemistry. As Coordinator, Dr. Weldegirma authored the experimental manuals, Experimental Organic Chemistry Laboratory Manual: CHM 2210L and CHM 2211L, to further the laboratory curriculum. Proceeds from the sale of these manuals were donated to the Castle Student Research Conference. We would like to thank him for his generosity in support of the Castle Conference.

Judges

American Chemical Society Tampa Bay Section

Adam Hopkins, Ph.D.
Ron Huffman, Ph.D.

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Andrea N. McCray, Ph.D.

Moffitt Cancer Center

John Koomen, Ph.D.
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Arjan van der Vaart, Ph.D.
Solomon Weldegirma, Ph.D.
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Juanjuan Yin, Ph.D.

Thank you to all of our judges for donating your time today to promote research and collaboration!

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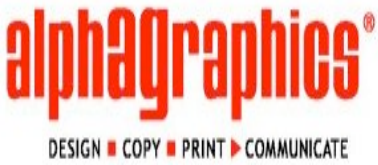

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This conference was supported, in part, by the University of South Florida Research & Innovation Internal Awards Program under Grant No. 0075435.

Graduate Talks Morning Session I (CHE 100)

Session Chair: Hasnaa Moutakki

8:30- 8:45 AM **HyunJoo Kil**
Synthesis of MTI-101 in Solution Phase

8:45- 9:00 AM **Daniel Dempsey**
Identification of an Arylalkylamine N-acyltransferase Enzyme that Catalyzes the Formation of Long-chain N-Acylserotonins and N-Acyldopamines

9:00- 9:15 AM **Arthur Maknenko**
A Two Step Synthesis of β-ester Glycolipid Mimics via Boron Trifluoride Etherate

9:15- 9:30 AM **Break**

9:30- 9:45 AM **Danielle Demers**
An Epigenetics Based Fungal Metabolite Screening Program for Antibacterial Lead Compounds

9:45- 10:00 AM **Yong Wang**
Asymmetric Olefin Cyclopropanation with Tosylhydrazones as Precursors of Donor-Substituted Diazo Reagents via Co(II)-Based Metalloradical Catalysis

Graduate Talks Morning Session II (CHE 111)

Session Chair: Parker Hutha

8:30- 8:45 AM **Justin White**
Quantum Mechanical and Molecular Mechanical Study Reveals Aromaticity to be a Driving Force of 1-Deoxy-d-xylulose 5-phosphate Synthase Activation

8:45- 9:00 AM **Mona Doshi**
Composite Conducting Polymer/Fullerene Nanobioprobes for Inducing Oxidative Stress in Cancer Cells Through Electron/Energy Transfer, and Their Application in Photodynamic Therapy

9:00- 9:15 AM **Fiona Kearns**
Computational Ecology: Elucidating Novel Chemical Defense Mechanisms of Antarctic Sea Sponges

9:15- 9:30 AM **Break**

9:30- 9:45 AM **Aleksandra Karolak**
Novel Coarse-Grained Model for Molecular Dynamics Simulations of DNA

9:45- 10:00 AM **Li Ye**
Investigating Student Responses Using an Open-Ended Assessment Technique to Examine Concept Retention in General Chemistry

Graduate Talks Afternoon Session I (CHE 100)

Session Chair: Danielle Demers

3:15- 3:30 PM **Qigan Cheng**
Asymmetric Olefin Cyclopropanation with α-Halodiazoacetates via Co(II)-Based Metalloradical Catalysis: Enantioselective Construction of Cyclopropyl Halides

3:30- 3:45 PM **Khanh Ha**
Challenges and Progress Toward Synthesis of Cyclic Peptide

3:45- 4:00 PM **Yaqiong Li**
Lipidated Cyclic gamma-AA Peptides Display Both Antimicrobial and Anti-inflammatory Activity

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

4:15- 4:30 PM **Iredia Iyamu**
Multi-Fragment Screening of Protein-Protein Interaction Modulators via Sulfo-Click Kinetic Target-Guided Synthesis

4:30- 4:45 PM **Chris Witowski**
New Secondary Metabolites Produced Via Co-cultures of a Marine Derived Bipolaris sp. Fungus

4:45- 5:00 PM **Ali Hussain**
Design and the Synthesis of Novel Water-Soluble Pseudo-Cyclodextrin Resorcin[4]arenes (CDR's) and their Application in Thiocyanations in Water

Graduate Talks Afternoon Session II (CHE 111)

Session Chair: Jacqueline Fries

3:15- 3:30 PM **Tony Pham**
Interpreting the Inelastic Neutron Scattering Spectra For Hydrogen in a Metal-Organic Framework

3:30- 3:45 AM **Luisana Astudillo**
Extended Termini in Cytoglobin Facilitate Association of 1,8-ANS and Lipids

3:45- 4:00 PM **Siqi Sun**
Preparation of Fe_3O_4/Ag Nanoparticles for Magnetic Separation and SERS Application

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

4:15- 4:30 PM **Yujuan Liu**
Motivation Toward Chemistry in Preparatory and Introductory College Chemistry Courses in Australia

4:30- 4:45 PM **Monica Mion Cook**
Endocrine-Disrupting Compounds: Exploring Solutions to Environmental Pollution

4:45- 5:00 PM **Adam Hogan**
Investigating Repulsion and Dispersion Potentials

The Barbara and Dean F. Martin Poster Session
CHE 103
Session Chair: Elizabeth Yancy

Graduate:	Group GP	All Disciplines

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

Undergraduate:	Group I	Organic (OR-01 – OR-14)
	Group II	Organic (OR-15 – OR-21), Analytical (AN-1 – AN-4), and Inorganic (IN-1 – IN-4)

The Solomon T. Weldegirma Poster Session
CHE 101A
Session Chair: Cole Cerrato

Undergraduate:	Group III	Biochemistry (BC-1 – BC-6), Computation (PC-1 – PC-9)
	Group IV	Natural Products (NP-1 – NP-14)

Graduate Talks

GT-01 **HyunJoo Kil**[1], Mark L. McLaughlin[1].
[1]Department of Chemistry, University of South Florida.

Synthesis of MTI-101 in Solution Phase

The β-hairpin peptide called as MTI-101 already showed good bioactivity against multiple myeloma (MM). For the next level of bio-study, the considerable amount of a β hairpin peptide was demanded. In order to make the substantial β-hairpin peptide, the solution phase peptide synthesis was chosen instead of the solid phase peptide synthesis because of the cost-effect. Two methodology were tried for the solution-phase peptide synthesis: (1) segment ligation and (2) continuous synthesis.

GT-02 **Daniel Dempsey**[1], Kristen A. Jeffries[1], Anne Marie Carpenter[1], Santiago Rodriguez Ospina[1], David J. Merkler[1].
[1]Department of Chemistry, University of South Florida.

Identification of an Arylalkylamine N-acyltransferase Enzyme that Catalyzes the Formation of Long-chain N-acylserotonins and N-acyldopamines

Fatty acid amides are an emerging class of cell signaling lipids that consist of N-acylarylalkylamides, N-acylethanolamines, N-acyl amino acids, N-monoacylpolyamines, and primary fatty acid amides. The N-acylarylalkylamides consist of the long-chain N-acyldopamines and N-acylserotonins, in which N-arachidonyldopamine was found to have a physiological role in pain perception, locomotion, and regulation of body temperature. Biosynthesis of these important lipids has remained elusive; however, there are data suggesting that these metabolites are formed by the conjugation of a fatty acid to the arylalkylamine. We have screened eight putative arylalkylamine N-acyltransferase like enzymes (AANATL) from D. melanogaster, and identified an enzyme that is consistent with this chemistry, AANATL2, that catalyzes the formation of long-chain N-acyldopamines and N-acylserotonins from the corresponding acyl-CoA and arylalkylamine substrates. Herein, we define the kinetic mechanism, elucidate structure-function relationships, and report data which led to a proposed chemical mechanism for D. melanogaster AANATL2.

GT-03 **Arthur Maknenko**[1], Kirpal S. Bisht[1].
[1]Department of Chemistry, University of South Florida.

A Two Step Synthesis of β-ester Glycolipid Mimics via Boron Trifluoride Etherate

Amphiphilic glycolipids display a variety of cellular functions, but are difficult to synthesize via a limited step scheme due to their chemical complexity. Mimics of these compounds can be prepared from cheap starting materials and investigated to determine their surfactant qualities. A straightforward preparation of β-glycolipid mimics in moderate yield via a short sequence boron trifluoride and peracetate deprotection scheme was achieved.

GT-04 **Danielle Demers**[1,2], Matthew Knestrick[1,2], Renee Fleeman[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, University of South Florida.

An Epigenetics Based Fungal Metabolite Screening Program for Antibacterial Lead Compounds

Since the birth of the antibiotic era, microbial natural products have played a key role in the treatment of bacterial infections. Chemically diverse and largely under-studied, marine endophytic fungi represent a valuable source of natural products for an antibiotic screening program. Recent advances in epigenetic modification provide relatively inexpensive and facile culture enhancements to up-regulate and express previously silent biosynthetic pathways, thus exploiting the full chemical potential of these microorganisms. In the face of diminishing discovery of new antibiotics and increasing resistance, the clinically relevant ESKAPE pathogens present a panel of gram positive and gram negative pathogens to challenge with this chemical diversity. Herein we provide a progress update on our distinctive program in which mangrove endophytes are epigenetically modified and their extracts screened against each of the ESKAPE pathogens with the aim of discovering a potent lead compound for development into a novel antibiotic therapies

GT-05 **Yong Wang**[1], Xin Cui[1], Xin Wen[1], X. Peter Zhang[1].
[1]Department of Chemistry, University of South Florida.

Asymmetric Olefin Cyclopropanation with Tosylhydrazones as Precursors of Donor-Substituted Diazo Reagents via Co(II)-Based Metalloradical Catalysis

Metalloradical catalysis has emerged as a new and powerful approach for stereoselective construction of three-membered cyclopropane structures. By employing tosylhydrazones as stable alternatives for donor-substituted diazo reagents, the cobalt(II) complex of the D2-symmetric chiral porphyrin, 3,5-DitBu-Xu(2'-Naph)Phyrin, has shown to be an effective metalloradical catalyst for asymmetric cyclopropanation with donor-substituted carbene sources. The asymmetric cyclopropanation by [Co(3,5-DitBu-Xu(2'-Naph)Phyrin)] can be applied for a broad range of olefins, affording the corresponding cyclopropane derivatives in high yields with both excellent diastereo- and enantioselectivities. Furthermore, the Co(II)-catalyzed stereoselective cyclopropanation features a high level of functional group tolerance. This Co(II)-based metalloradical system represents the first catalytic system for highly asymmetric olefin cyclopropanation with donor-substituted carbene sources, allowing for efficient accesses of new types of optically active cyclopropanes that were difficult to be synthesized using existing methodologies.

GT-06 **Justin White**[1], H. Lee Woodcock[1].
[1]Department of Chemistry, University of South Florida.

Quantum Mechanical and Molecular Mechanical Study Reveals Aromaticity to be a Driving Force of 1-Deoxy-d-xylulose 5-phosphate Synthase Activation

1-deoxy-d-xylulose 5-phosphate (DXS) is a thiamine diphosphate (TDP) dependent enzyme that is the initial step of the non-mevalonate pathway for isoprenoid biosynthesis. DXS undergoes an activation step and produces a ylidic form of TDP; which requires a base to initiate. Two bases have been proposed based on mechanistic similarities to transketolase enzymes: a water or histidine. Quantum mechanical and molecular mechanical

techniques were used to calculate the barrier heights of the reactions employing either the histidine or water molecule. Furthermore, comparisons of the reactant and transition states were performed to determine differences in how each state is being stabilized. These comparisons revealed structural changes that were indicative of a novel driving force. Further investigation revealed aromaticity to be a significant factor in energetics of ylide formation.

GT-07 **Mona Doshi**[1], Alicja Copik[2], Andre J. Gesquiere[1,3,4].
[1]Department of Chemistry, University of Central Florida
[2]Department of Biomedical Sciences, University of Central Florida
[3]Department of Materials Science and Engineering, University of Central Florida
[4]Center for Research and Education in Optics and Lasers, University of Central Florida

Composite Conducting Polymer/Fullerene Nanobioprobes for Inducing Oxidative Stress in Cancer Cells Through Electron/Energy Transfer, and Their Application in Photodynamic Therapy

In this presentation, the development of composite conducting conjugated polymer/fullerene nanoparticles and the formation oxidative stress in cancer cells is discussed. Under irradiation with light, the conducting polymer MEH-PPV (Poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]) acts as a donor and PCBM (Phenyl C61 Butyric acid Methyl ester) acts as an acceptor to form charges which are dissipated via triplet energy transfer or electron transfer to oxygen to form high levels of Reactive Oxygen Species (ROS). The ROS produced inside the cells was confirmed by epiluminescence imaging with CellROX green reagent. Intrinsic cytotoxicity of the nanoprobes and the viability of cells after PDT were quantified by MTT assays. The nanoprobes were found to be not cytotoxic in dark. PDT experiments showed significantly low cell viability with necrotic and apoptotic differentiation in different cell lines. Due to their photophysical and photochemical properties the these nanoprobes can be made very useful in biophotonics and therapeutics.

GT-08 **Fiona Kearns**[1], Sai Lakshmana Vankayala[1], Bill J. Baker[1,2], H. Lee Woodcock[1].
[1]Department of Chemistry, University of South Florida.
[2]Center for Drug Discovery & Innovation, University of South Florida.

Computational Ecology: Elucidating novel chemical defense mechanisms of Antarctic Sea Sponges

A novel secondary metabolite, erebusinone, was isolated from the Antarctic sea sponge, Isodictya erinacea, by the Baker Research group in 2000; it was also shown to inhibit molting in arthropods. The structure of erebusinone was determined to be similar to xanthurenic acid, a known endogenous molt-inhibitor in arthopods. Xanthurenic acid is known to interrupt the synthesis of the molt inducing hormone, 20-hydroxyecdysone and we hypothesize erebusinone may also work by the same mechanism of action. The molting pathway is governed by a small set of P450 enzymes and due to a lack of isolated molting P450 crystal structures and sequences from marine crustaceans, experimentation has become difficult. An array of computational techniques (homology modeling, molecular dynamics simulations, binding site bioinformatics, and induced fit docking) have been employed to predict the 3D structures for two proteins (CYP315a1, CYP314a1) responsible for molting and their interaction with potential small molecule inhibitors.

GT-09 **Aleksandra Karolak**[1], Arjan van der Vaart[1].
[1]Department of Chemistry, University of South Florida

Novel Coarse-grained Model for Molecular Dynamics Simulations of DNA

We have developed an efficient, sequence-specific coarse-grained model to simulate the conformational motion of large double stranded DNA in molecular dynamics simulations. The DNA backbone is modeled by beads with DNA bases represented by sets of three beads, and bead positions are used to calculate the shift, slide, rise, roll, twist and tilt conformational step parameters of DNA. With these parameters, elastic deformation energies are calculated following Olson's harmonic model (Olson et. al., Proc. Natl. Acad. Sci. USA 95, 11163 (1998)). Specifics of the model and test simulations will be discussed.

GT-10 **Li Ye**[1], Scott Lewis[1].
[1]Department of Chemistry, University of South Florida.

Investigating Student Responses Using an Open-Ended Assessment Technique to Examine Concept Retention in General Chemistry

Creative Exercises are an open-ended student assessment technique where students are given a brief prompt, such as “a molecule of CH2O”. Students are then instructed to write as many statements as they can that are distinct, correct and relevant to the prompt and the course content. The intention is that Creative Exercises promote the linking of students’ concepts within a course. This presentation describes an investigation into the use of Creative Exercises as an instructional means for learning about students’ concept retention and uncovering student misconceptions. Creative Exercises were used as a regular student assessment in multiple first semester General Chemistry classes. Student responses were coded using an open-ended coding scheme with two raters. The analysis provides evidence that students were successfully applying prior knowledge toward recently presented topics. Novel student misconceptions were also found with implications on students’ understanding of limits of models.

GT-11 **Qigan Cheng**[1], Silke Evdokimov[1], Xue Xu[1], Jennifer Lee[1], Lukasz Wojtas[1], X Peter Zhang[1].
[1]Department of Chemistry, University of South Florida.

Asymmetric Olefin Cyclopropanation with α-Halodiazoacetates via Co(II)-Based Metalloradical Catalysis: Enantioselective Construction of Cyclopropyl Halides.

The cobalt(II) complex of the D2-symmetric chiral porphy-rin 3,5-DitBu-ChenPhyrin, [Co(P1)], has proven to be an effective catalyst for catalyzing asymmetric olefin cyclo-propanation with α-chlorodiazoacetates and α-bromodiazoacetates. The [Co(P1)]-mediated metalloradical cyclopropanation is suitable for a wide range of aromatic and aliphatic olefins with varied steric and electronic properties, providing the corresponding halogenated cyclopropanes in high yields with excellent diastereo- and enantioselectivity.

GT-12 **Khanh Ha**[1], Sadra Hamedzadeh[1], Ryan Quiñones[1], Grant Simpson[1], Amir Nasajpour[1], Jay McDaniel[1], Jocelyn Macho[1], Alan Katritzky[1].

[1]Center for Heterocyclic Compounds, University of Florida.

Challenges and Progress Toward Synthesis of Cyclic Peptide

Cyclic peptides are important targets for the development of synthetic protocols because peptide macrocycles have found applications that range from drug discovery to nanomaterials. New and improved strategies lead to more efficient synthesis of complex peptide targets, opening the way to both new drug candidates and a deeper understanding of the intimate relation between sequence, conformation and properties. Despite recent progress and the arsenal of reagents available, synthesis of medium ring-sized cyclo-peptide remains challenging: complex targets and regulatory authority constraints in terms of purity for drugs are continuously stimulating chemists to improve and rethink synthetic approaches. Reducing the no. of steps is usually a synonym of better yields and ease of purifn., which explains the success of convergent peptide synthesis. We now report the development of synthetic methods and approaches targeting medium-sized cyclic peptides including: dimerization-macrocyclization, conformationally assisted marco-cyclization, intramol. Staudinger ligation.

GT-13 **Yaqiong Li**[1], Christina Smith[2], Haifan Wu[1], Shruti Padhee[1], Hubert Yin[2], Jianfeng Cai[1].
[1]Department of Chemistry, University of South Florida

[2]University of Colorado, Boulder.

Lipidated Cyclic gamma-AApeptides Display Both Antimicrobial and Anti-inflammatory Activity

The lipidated cyclic compounds we made have potent antibacterial activity against clinically relevant Gram positive and gram negative bacteria. Besides, they harness the immune response and inhibit lipopolysaccharide (LPS) activated Toll-like Receptor 4 signaling, suggesting that lipidated cyclic gamma-AApeptides have dual roles as novel antimicrobial and anti-inflammatory agents.

GT-14 **Iredia David Iyamu**[1], Katya Nacheva[1], David Flanigan[1], Sameer Kulkarni[1], Megan Barber[1], Wang Hong-Gang[2], Niranjan Namelikonda[1], Roman Manetsch[1]
[1]Department of Chemistry, University of South Florida.

[2]Penn State College of Medicine.

Multi-Fragment Screening of Protein-Protein Interaction Modulators via Sulfo-Click Kinetic Target-Guided Synthesis.

Although protein-protein interactions (PPIs) are considered to possess significant biological importance, identification of small PPI modulators remains challenging. Several fragment-based approaches have been developed to identify specific ligands with good ligand efficiencies, but failure to provide insight into efficient fragment evolution has made the lead discovery and development process cumbersome and complicated. Herein, we report the development of a fragment evolution platform, known as kinetic target-guided synthesis (TGS), that generates only biologically active compounds. In kinetic TGS, the biological target is actively engaged in the irreversible assembly of its own inhibitory bidentate ligand from a pool of smaller reactive fragments. The sulfo-click reaction between fragments bearing a thio acid or sulfonyl azide was successfully employed by the Manetsch laboratory for a kinetic TGS approach targeting the PPI targets Bcl-XL and Mcl-1. Herein, we discuss the

optimization of the sulfo-click chemistry based kinetic TGS approach focusing on significant improvements related to throughput and data quality.

GT-15 **Chris Witowski**[1,2], Riley Bednar[1,2], Renee Fleeman[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 Secondary Metabolites Produced Via Co-cultures of a Marine Derived Bipolaris sp. Fungus

Microbial natural products remain a potent source of anti-infectives in modern drug discovery. Competitive interactions are a prominent factor in secondary metabolite production, however, typical solitary culture techniques do not access the full chemical potential found in complex microbial environments. Recently, microbial co-cultures have been shown to increase production of known compounds and induce production of novel secondary metabolites. Crude extracts from a Bipolaris sp. fungus isolated from the Caribbean Sea displayed activity against Aspergillus niger, a common fungal contaminant. A scale-up was initiated on agar plates to co-culture the two organisms for targeted antibiotic production. Each plate was excised into three regions, the zone of inhibition and the mycelium of each fungus, to determine the origin of metabolites. Separation of the Bipolaris material yielded known antifungal compounds as well as two new natural products.

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

Design and the Synthesis of Novel Water-Soluble Pseudo-Cyclodextrin resorcin[4]arenes (CDR's) and their Application in Thiocyanations in Water

A family of two tetra-valent and an eight arms octopus like structure water-soluble pseudo-cyclodextrin resorcin[4]arenes (CDRs) were designed and envisioned by decorating synthesized resorcin[4]arene intermediates with β-D-glucopyranosides via Cu(I)-catalyzed Azide-Alkyne Cycloaddition (CuAAC). The utility of CDRs have been demonstrated as a phase transfer catalysts for environmental green thiocyanation reactions in water. Benzyl bromide was chosen as a candidate in the presence of KSCN in water to optimize the thiocyanation reaction condition and to study the conversion (%) with and without CDRs within 5-20min. Furthermore, thiocyanation in the presence of CDR1 for different alkyl/aryl bromides with KSCN in water were successfully achieved resulting in the desired thiocyanate products in high yield within short period of time reaction.

GT-17 **Tony Pham**[1], Katherine A. Forrest[1], Juergen Eckert[1], Brian Space[1].
[1]Department of Chemistry, University of South Florida

Interpreting the Inelastic Neutron Scattering Spectra For Hydrogen in a Metal-Organic Framework

Simulations of hydrogen sorption were performed in a metal-organic framework (MOF) in order to identify the favorable sorption sites in the material. For each site considered, the two-dimensional quantum rotational levels for a single hydrogen molecule about that site were calculated. The calculated transitions were in good agreement to those that were observed in the inelastic neutron scattering (INS) spectra for hydrogen in the MOF. As a result, the

assignment of the peaks in the INS spectra for the MOF has been made, leading to a comprehensive interpretation of the spectra.

GT-18 **Luisana Astudillo**[1], Khoa Pham[1], Antonija Tangar[1], Jaroslava Miksovska[1].
[1]Department of Chemistry & Biochemistry, Florida International University.

Extended Termini in Cytoglobin Facilitate Association OF 1,8-ANS and Lipids

Cytoglobin (Cygb) is a recently discovered heme protein belonging to the family of hexa-coordinate hemoglobins that is over-expressed under fibrosis conditions and down-regulated in some types of cancer. Lipid binding to Cygb leads to a conformational transition from hexa- to penta-coordinate heme iron, suggesting a role of Cygb in lipid signaling. To understand the mechanism of Cygb interactions with lipids, we characterized the interactions of 1,8-ANS and Cygb using fluorescence spectroscopy and isothermal titration calorimetry. Cygb binds 1,8-ANS with moderate affinity (Kd=20 μM), whereas a truncated form of Cygb that does not contain the extended N- and C-termini does not associate to 1,8-ANS. Oleate binding to Cygb-ANS complex decreases 1,8-ANS emission intensity indicating competition between the lipid and ANS for Cygb binding site. Molecular docking studies suggest that 1,8-ANS and oleate bind at a site located at the extended N-terminus in Cygb.

GT-19 **Siqi Sun**[1], Xiao Li[1].
[1]Department of Chemistry, University of South Florida.

Preparation of Fe_3O_4/Ag Nanoparticles for Magnetic Separation and SERS Application

Melatonin played an important role in Alzheimer's disease as an antioxidant and as a neuroprotector. This study focused on development of the novel sensitive substrate of Fe_3O_4@Ag core-shell magnetic nanoparticles for melatonin detection. Fe_3O_4@Ag nanoparticles were synthesized, and their surface morphology and structure were characterized using TEM. Fe_3O_4 nanoparticles with size of 10 nm were synthesized as the core. The thickness of Ag shell can be tuned through the adjustment of the molar ratio between Fe_3O_4 to Ag_2SO_4. The sensitivity and reproducibility of the substrates were tested by detecting rhodamine 6G (R6G), a common SERS probe molecule. More importantly, this substrate showed big advantages of extraction and enrichment of low concentration R6G samples which could further lower the detection limit. This study provides a potential method for analysis of trace amount of melatonin in complex biological samples by combining separation and detection.

GT-20 **Yujuan Liu**[1], Daniel Southam[2], Jennifer E. Lewis[1].
[1]Department of Chemistry, University of South Florida
[2]Department of Chemistry, Curtin University, Perth, Australia

Motivation Toward Chemistry in Preparatory and Introductory College Chemistry Courses in Australia

Motivation is an important variable in the affective domain, as motivation is found to be an important factor in student achievement and retention. According to Self-Determination Theory, motivation interplays with the social environment, and we anticipate that students will be more intrinsically motivated in higher-level chemistry courses. The purpose of the study is to examine student motivation toward chemistry in a preparatory- and introductory-level college courses in Australia using Academic Motivation Scale – Chemistry. In both courses a student-centered teaching strategy was implemented. Evidence was collected for response process and internal structure validity, and internal consistency reliability was also examined. The results showed that students scored higher on

all extrinsic and intrinsic motivation subscales in the higher-level course, with small to medium effect sizes. Such results encourage us to investigate the important factors for the changes, which could inform curriculum design decisions for instructors who care about student motivation.

GT-21 **Monica Mion Cook**[1], Leon Hardy[2].
[1]College of Marine Science, University of South Florida
[2]Department of Biological Sciences, University of South Florida

Endocrine-Disrupting Compounds: Exploring Solutions to Environmental Pollution

The presence of estrogenic endocrine-disrupting compounds (EDCs) in the environment has become a major topic in marine pollution. EDCs are found at low concentrations throughout the environment, but even low concentrations can negatively affect terrestrial or aquatic wildlife. The effects of EDCs on wildlife have been well documented. In mitigating the environmental impact of EDCs, two things become very important: 1. Techniques for removing EDC pollutants from water and 2. Tools for determining the molecular basis of endocrine disruption. Here we will describe a removal technique called electrocoagulation (EC). We will then examine the value in utilizing computer models to determine the structural features of EDCs that become so important in binding to an endocrine receptor.

GT-22 **Adam Hogan**[1], Brian Space[1].
[1]Department of Chemistry, University of South Florida.

Investigating Repulsion and Dispersion Potentials

Repulsion and dispersion accounts for the majority of the interaction energy between most molecules. It is therefore important to reproduce these energies as accurately as possible for use in computational simulations. For example the results of a gas sorption simulation in Metal-organic frameworks (MOFs) can be highly dependent on the force field chosen. This talk will focus on comparing different potential energy forms to high level ab initio. A method for determining the dispersion energy based on SAPT and Coupled Cluster energies will be presented. Another method for determining dispersion coefficients from electronic density will be also presented. These methods will then be applied to create a physically meaningful classical force field for hydrogen.

The Barbara and Dean F. Martin Poster Session Abstracts

GP-01 **Jacqueline von Salm**[1], Nerida G. Wilson[2], Brian A. Vesley[3], Dennis E. Kyle[3], Jason Cuce[1], Bill J. Baker[1].
[1]Department of Chemistry, University of South Florida
[2]Western Australian Museum
[3]Department of Global Health, University of South Florida

Shagenes A & B, Tricyclic Sesquiterpenes Produced by an Undescribed Antarctic Octocoral

Here we present the isolation and characterization of two novel tricyclic sesquiterpenoids, shagenes A and B, with an unexampled carbon skeleton. These compounds were produced by a genetically intriguing cold-water octocoral collected at approximately 180 meters depth along the Scotia Arc. Phylogenetic analysis using the octocorallian mitochondrial mismatch repair (mtMutS) gene place this organism outside of known Octocorallia families. One- and two-dimensional NMR spectroscopy as well as high-resolution mass obtained from a GC-MS QToF provided the data necessary to characterize the planar structures of the compounds. Relative stereochemical configurations are based on ROESY experiments. Exploration of the bioactivity of shagenes A and B found shagene A active against the parasite that causes visceral leishmaniasis, Leishmania donovani with no cytotoxicity against the mammalian host. No bioactivity was observed in shagene B eluding to the importance of the methoxy substituent at position C-8.

GP-02 **Yaqiong Li**[1], Christina Smith[2], Haifan Wu[1], Shruti Padhee[1], Hubert Yin[2], Jianfeng Cai[1].
[1]Department of Chemistry, University of South Florida
[2]University of Colorado, Boulder.

Lipidated Cyclic gamma-AApeptides Display Both Antimicrobial and Anti-inflammatory Activity

We reported the lipidated cyclic gamma-AApeptides that have potent antimicrobial activity against clinically relevant gram positive and gram negative bacteria, many of which are resistant to conventional antibiotics. Besides, the compounds we made harness the immune responses and inhibit LPS activated Toll-like Receptor 4 signalling, suggesting that the lipidaated cyclic gamma-AApeptides have dual roles as novel antimicrobial and anti-inflammatory agents.

GP-03 **Haifan Wu**[1], Yaqiong Li[1], Ge Bai[1], Chuanhai Cao[2], Jianfeng Cai[1].
[1]Department of Chemistry, University of South Florida
[2]College of Pharmacy, University of South Florida

γ-AApeptide-based Unnatural Small-Molecule Ligands

A novel class of Gamma-AApeptide one-bead-one-compound (OBOC) library was prepared using split-and-pool methods. This 192,000-member Gamma-AApeptide library was demonstrated to be a valuable source of novel protein/peptide ligands by identifying a small Gamma-AApeptide HW-155-1 that can effectively prevent and disassemble Aß40 aggregation. This is not only the first report of Gamma-AApeptide based combinatorial library; in addition, HW-155-1 is also one of the most potent small molecules that disrupt Aß aggregation. Our results show that Gamma-AApeptides are ideal candidates for the identification and development of novel ligands and drug candidates.

GP-04 **Aleksandra Karolak**[1], Arjan van der Vaart[1].
[1]Department of Chemistry, University of South Florida

Novel Coarse-Grained Model for Molecular Dynamics Simulations of DNA

We have developed an efficient, sequence-specific coarse-grained model to simulate the conformational motion of large double stranded DNA in molecular dynamics simulations. The DNA backbone is modeled by beads with DNA bases represented by sets of three beads, and bead positions are used to calculate the shift, slide, rise, roll, twist and tilt conformational step parameters of DNA. With these parameters, elastic deformation energies are calculated following Olson's harmonic model (Olson et. al., Proc. Natl. Acad. Sci. USA 95, 11163 (1998)). Specifics of the model and test simulations will be discussed.

GP-05 **Sreya Mukherjee**[1], Wesley Brooks[1], Wayne Guida[1].
[1]Department of Chemistry, University of South Florida.

Drug Discovery on STIM1

Calcium ions play important roles in intracellular signaling, protein folding, enzyme activation and apoptosis. Following signal cascades triggered by a variety of surface receptors, calcium stored in the endoplasmic reticulum (ER) is released into the cytosol. Stromal Interaction Molecule 1 (STIM1) an ER transmembrane protein, is activated by a drop in ER calcium. Activated STIM1 interacts with ORA1, a plasma membrane protein, to open ORAI1 calcium channels which allows entry of extracellular calcium to fully activate calcium dependent processes. Eventually calcium is sequestered and homeostasis is restored ready for another triggering signal. Dysregulation of this calcium flux has been reported in cancers, autoimmune diseases and other diseases. The key role of STIM1 early in calcium flux makes it an interesting target in drug discovery. Herein, computational techniques were used to understand the mechanistic role of STIM1 and virtual screening is in process to discover potential inhibitors of STIM1 activity.

GP-06 **Geoffrey M. Gray**[1], Arjan van der Vaart[1].
[1]Department of Chemistry, University of South Florida

The Increased Affinity and Decreased Selectivity of the HPV6 E2 ΔLL Mutant Stems from a Decrease in DNA Bending in the Mutant Complex

The human papillomavirus type 6 E2 protein binds the 5'-AACCG-NNNN-CGGTT-3' DNA consensus sequence, where NNNN is a linker region. The wild-type (WT) protein only binds A/T rich linker regions in a binding process kinetically characterized by a fast phase followed by a slow phase, whereas the E2ΔLL mutant shows enhanced affinity for both A/T and G/C rich linker sequences with a significantly sped up fast phase. To rationalize these observations, we performed long molecular dynamics simulations of the WT bound to DNA with AATT and CCGG linkers, and of E2ΔLL bound to the same sequences. It was found that the DNA bending angle was decreased to 25° for both E2ΔLL-DNA complexes, while the bending angle was 60° in the WT complexes. The decreased bending angle lowers the DNA distortion energy in the mutant complexes, explaining the increased binding affinity of the E2ΔLL protein along with the kinetic results.

GP-07 **Yong Wang[1]**, Xin Cui[1], Xin Wen[1], X. Peter Zhang[1].
[1]Department of Chemistry, University of South Florida.

Asymmetric Olefin Cyclopropanation with Tosylhydrazones as Precursors of Donor-Substituted Diazo Reagents via Co(II)-Based Metalloradical Catalysis

Metalloradical catalysis has emerged as a new and powerful approach for stereoselective construction of three-membered cyclopropane structures. By employing tosylhydrazones as stable alternatives for donor-substituted diazo reagents, the cobalt(II) complex of the D2-symmetric chiral porphyrin, 3,5-DitBu-Xu(2'-Naph)Phyrin, has shown to be an effective metalloradical catalyst for asymmetric cyclopropanation with donor-substituted carbene sources. The asymmetric cyclopropanation by [Co(3,5-DitBu-Xu(2'-Naph)Phyrin)] can be applied for a broad range of olefins, affording the corresponding cyclopropane derivatives in high yields with both excellent diastereo- and enantioselectivities. Furthermore, the Co(II)-catalyzed stereoselective cyclopropanation features a high level of functional group tolerance. This Co(II)-based metalloradical system represents the first catalytic system for highly asymmetric olefin cyclopropanation with donor-substituted carbene sources, allowing for efficient accesses of new types of optically active cyclopropanes that were difficult to be synthesized using existing methodologies.

GP-08 **Ning Ma[1],** Elana M.S. Stennett[2], Marcia Levitus[2], Arjan van der Vaart[1].
[1]Department of Chemistry, University of South Florida.
[2]Arizona State University.

Photophysical and Dynamical Properties of Doubly Linked Cy3 – DNA Constructs

Photophysical measurements and molecular dynamics simulations are reported for doubly linked Cy3–DNA constructs. It is shown that trans-to-cis isomerization and intercalation occur, with low barriers for intercalation. These findings indicate the unexpected occurrence of complex dynamics for the highly rigidified construct, which complicate its potential use as molecular ruler.

GP-09 **David Butcher[1]**, Jaroslava Miksovska[1].
[1]Department of Chemistry & Biochemistry, Florida International University.

DNA i-motif Probed by Photoacoustic Calorimetry.

The intercalated motif (i-motif) occurs in the C-rich strand of regulatory regions of the genome and human telomere. Its formation is favored at acidic pH (<6). The steps of i-motif folding are presently not well characterized. Photoacoustic calorimetry (PAC) has been used with a 2-nitrobenzaldehyde pH-jump technique to characterize thermodynamic and kinetic parameters of protonation and intramolecular folding of an oligomer (5'-[CCCTAA]3CCC-3') into the i-motif on fast timescales (~50 ns to 10 μs). Two kinetic steps were resolved, the first one corresponds to proton release and subsequent protonation of cytosines in the DNA strand within 50 ns. The second corresponds to folding of the i-motif with a lifetime of 300 ns. We determine ΔH and ΔV for the fast step to be -104 kcal mol-1 and -13.6 mL mol-1. For the slow step, ΔH and ΔV were observed to be 234 kcal mol-1 and 9.5 mL mol-1.

GP-10 **Iman Hajinezhad[1],** Sean Michael[1], Dimitra Keramisanou[1], Ioannis Gelis[1].
[1]Department of Chemistry, University of South Florida.

Molecular Insights Into The Mechanism of Chaperone-Kinase Recognition

Cdc37 is a key component of the Hsp90 chaperone machinery necessary for protein kinase folding, and thus it provides an attractive chemotherapeutic target. How Cdc37 recognizes nascent, misfolded or partially folded client kinase proteins and facilitates their recruitment to Hsp90 is poorly understood. Due to the dynamic nature of the interaction and the low conformational stability of the substrates, solution-state NMR is particularly well-suited to provide atomic resolution insights. Coupled with the characterization of binding energetics from isothermal titration calorimetry, NMR analysis may lend insight into the first and most decisive step of HSP90 mediated kinase chaperoning.

GP-11 **Benjamin Eduful[1]**, Catherine Costa[1], Vesely Brian[2], Azhari Ala[2], James Leahy[1].
[1]Department of Chemistry, University of South Florida.
[2]Deapartment of Public Health, University of South Florida.

Synthesis of a Novel Class of Antileishmaniasis Agents

Leishmaniasis is a parasitic disease transmitted by 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). The disease presents in three main forms: Cutaneous (most common); Visceral (most severe form) and Mucocutaneous (most destructive form) Leishmaniasis. Antimony, Amphotericin or Pentamidine are currently used as treatments for the disease but none is particularly effective; hence the need to develop highly effective new drugs. It is known that Heat Shock Protein 90 (Hsp90) is the most abundant protein 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 molecular scaffold.

GP-12 **Zachary Shultz[1]**, Ali Siddiqui[1], James Leahy[1].
[1]Department of Chemistry, University of South Florida.

Total Synthesis and SAR of Membranolide-A to Determine Bioactivity against Resistant Bacteria

Antibacterial resistance is occurring at an alarming rate with the continual occurrence of drug resistant pathogens that have been plaguing society throughout the last century. As of now, drug resistance is developing faster than the discovery of new drugs. The increasing need for new anti-infectives has led to the discovery of natural products such as the family of Membranolides, which were isolated from Antarctic sea sponge Dendrilla membranosa, that show promising bioactivity against Methicillin resistant strains of Staphylococcus aureus (MRSA) and Vancomycin-resistant enterococci (VRE). Model compounds of Membranolide-A will be synthesized in a structural activity relationship (SAR) study. A total synthesis will also be performed utilizing novel methodology such as one-pot Mitsunobu-Claisen rearrangements to introduce stereocenters in order to determine the currently unknown absolute stereochemistry of the natural product. Optimization of Membranolide-A will also be performed by synthesizing a variety of analogs to explore substituent modifications throughout the Membranolide core.

GP-13 **Walter Gonzalez**[1], Jaroslava Miksovska[1].
[1]Department of Chemistry & Biochemistry, Florida International University.

Dynamics and Thermodynamics of Calcium Induced Transition in DREAM Protein Using Photothermal Beam Deflection

Here we show the implementation of photothermal beam deflection (PBD) as a useful label free technique for the measurement of millisecond and sub-millisecond kinetics. Moreover, by taking advantage of the photosensitive calcium chelating compound DM-nitrophen, we have been able to photo trigger the release of calcium and consequent binding to four DREAM constructs. The PBD traces for photolysis of Ca2+DMNP show a fast 300 μs decay, whereas upon addition of DREAM(65-256) an additional slow phase with a decay of 1 ms can be resolved. Moreover, a construct lacking the first 161 amino acids shows a slower 5 ms decay. The differences in kinetics can be correlated with the oligomerization transition associated with each construct, where DREAM(65-256) undergoes a tetramer to dimer and DREAM(161-256) a monomer to dimer transition upon calcium binding. The slow transition is measured to be endothermic with a concomitant volume expansion.

GP-14 **Khoa Pham**[1], Jaroslava Miksovska[1].
[1]Department of Chemistry & Biochemistry, Florida International University.

Molecular Mechanism of DREAM and Presenilin-1 Interactions

One obstacle in Alzheimer's disease (AD) therapy development is to better understand the molecular mechanism of AD associated protein, presenilin (PS), interacted with its partner(s). Here, we discuss the interaction of DREAM with a short segment of PS1 C-terminus (helix-9). Using fluorescence anisotropy, it is determined that association of DREAM to helix-9 is calcium dependent (Kd(Ca^{2+}) ~ 0.8 μM, whereas Kd(Apo) ~ 183 μM). The helix-9 binds to C-terminal domain of DREAM protein with Kd ~ 11 μM. Moreover, a single calcium ion binding to EF-3 of DREAM can regulate DREAM and helix-9 interaction. The association of DREAM to helix-9 results in slower depolarization of DREAM-helix-9 complex. The rotational correlation time is found to be Φ = 22.5 ns. Our kinetics data demonstrated that association of DREAM to helix-9 is temperature and concentration dependent. The activation barrier is found to be Ea ~15 kcal•mol-1 suggesting for the DREAM conformational changes that decrease the flexible mobility of its binding site for helix-9. These results suggest that DREAM binds to PS1 in a dimeric form and the formation of inter-protein complex is regulated by Ca2+.

GP-15 **Ken Kull**[1], **Alejandro Rivera Nicholls**[1], Julie P. Harmon[1].
[1]Department of Chemistry, University of South Florida.

Configuration-Characteristics Relationship of Polyimides Based on Pyromellitic Dianhydride, an Aromatic Diamine and Short-Chain Aliphatic Diamines for

Polyimides are a class of high temperature resistant thermoplastic polymers. They are most frequently used because of their thermal stability and good mechanical properties. The nature of these types of polyimides makes them very rigid with a very high melting point which limits the processing options. We have designed a series of polyimides that will have a lower melting point using a range of molecular weight aliphatic diamines (Jeffamines D230, D400, D2000 and D4000). A common dianhydride, pyromellitic dianhydride (PMDA) is reacted with various aliphatic diamines to produce lower melting, flexible polymers. FTIR, TGA, DSC and molecular weight are

reported for all polymers studied. The synthesis, physical properties and applications of advanced polyimide materials are described.

GP-16 **Garrett Craft**[1], **Cody Haynes**[1], Julie Harmon[1].

[1]Department of Chemistry, University of South Florida.

Advancing Composite Materials for Biological Applications

In this study, a hydrogel system and a metal organic secondary building unit (SUB) will be synthesized for applications towards constructing tunable drug delivery platforms and improved biocompatible materials. Hydrogels are a family of hydrophilic materials which can swell to enormous extents in aqueous environments yet remain undissolved, with their structure maintained via physical or chemical crosslinking. The extraordinarily high content of sorbed water along with high porosity makes these structures one of the most lifelike synthetic materials in existence, with their swelling and diffusion characteristics being tunable with the use of composites and copolymeric compositions.

GP-17 **Parker Huhta**[1], Christi Whittington[1], Randy Larsen[1].
[1]Department of Chemistry & Biochemistry, Florida International University.

Thermodynamics of Nitric Oxide Photorelease from Sodium Nitroprusside

Nitric oxide (NO) is a ubiquitous signaling molecule in mammalian biology with a broad array of physiological functions. NO has been utilized clinically due to its ability to palliate hypoxic conditions through activation of the soluble guanlylyl cyclase pathway which stimulates vasodilation in vivo. Sodium Nitroprusside (SNP) is a potent NO donor that is widely used in the treatment of hypertensive crises and acute congestive heart failure. NO release can be photoinitiated, where using wavelength greater than 480nm yields free NO and the H_2O bound pentacyanoferrate(III). Knowledge of the thermodynamic profile and mechanism of NO release from SNP is crucial to developing new drug therapies for hypoxia. In this study, Photoacoustic Calorimetry is utilized to determine the enthalpy and volume changes associated with NO photorelease from SNP and subsequent H_2O binding. In addition, experimental and computational data will be presented which elucidate the photorelease mechanism.

GP-18 **Ranjani Muralidharan**[1], **Parker Huhta**[1], Santiago Sandi-Urena[1], Patricia Muisener[1].

[1]Department of Chemistry, University of South Florida.

The Academic Research Experience for Undergraduates Program

Since 2005, the Academic Research Experience for Undergraduates Program (REU) in the Department of Chemistry has actively engaged undergraduate students in a hands-on research experience. The program works by matching students with faculty mentors by area of interest and with the help of graduate mentors, supervise undergraduates in research projects. The REU also functions to educate students by providing workshops in the areas of abstract writing, presentation skills and graduate school admissions. In addition, students are invited to participate in special seminars given by chemistry faculty. The goals of the REU program are too enhance the student learning experience through hands on work, and cultivate a lifelong appreciation and knowledge of

research in chemistry. The REU program strives to inspire students in their career goals and equip them with the tools to excel in all their future endeavors.

GP-19 **Danielle Demers**[1,2], **Matthew Knestrick**[1,2], Renee Fleeman[3], Lindsey N. Shaw[3], Bill J. Baker[1,2].
[1]Department of Chemistry, University of South Florida.
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[3]Department of Cell Biology, University of South Florida.

An Epigenetics Based Fungal Metabolite Screening Program for Antibacterial Lead Compounds

Since the birth of the antibiotic era, microbial natural products have played a key role in the treatment of bacterial infections. Chemically diverse and largely under-studied, marine endophytic fungi represent a valuable source of natural products for an antibiotic screening program. Recent advances in epigenetic modification provide relatively inexpensive and facile culture enhancements to up-regulate and express previously silent biosynthetic pathways, thus exploiting the full chemical potential of these microorganisms. In the face of diminishing discovery of new antibiotics and increasing resistance, the clinically relevant ESKAPE pathogens present a panel of gram positive and gram negative pathogens to challenge with this chemical diversity. Herein we provide a progress update on our distinctive program in which mangrove endophytes are epigenetically modified and their extracts screened against each of the ESKAPE pathogens with the aim of discovering a potent lead compound for development into a novel antibiotic therapies

GP-20 **Yuri Pevzner**[1], Daniel N. Santiago[1], Wesley H. Brooks[1], Wayne C. Guida[1], H. Lee Woodcock[1].
[1]Department of Chemistry, University of South Florida.

Development of the CHARMM Interface and Graphics Web Potal as a Platform for Computer Aided Drug Design

Web-based front end interfaces to scientific applications are important tools that allow researchers to utilize a broad range of software packages with just an Internet connection and a browser. One such interface, CHARMMing (CHARMM interface and graphics), allows researchers to take advantage of the functionality of the powerful and widely used molecular software package CHARMM. CHARMMing incorporates tasks such as molecular structure analysis, energy minimization, molecular dynamics and other techniques commonly used by computational life scientists. We are extending CARMMing's capabilities to include common drug discovery tasks that include docking, virtual screening and virtual target screening. As part of this undertaking docking and scoring protocols that utilize the latest CHARMM protein, nucleic acid and small molecule force fields are being developed and evaluated.

GP-21 **Xin Wen**[1], Xin Cui[1], Yong Wang[1], Li-Mei Jin[1], X. Peter Zhang[1].
[1]Department of Chemistry, University of South Florida.

Asymmetric Intramolecular C-H Alkylation using Tosylhydrazones as Alternatives for Donor-type Diazo Reagents via Co(II)-based Metalloradical Catalysis

Catalytic asymmetric systems for C–H functionalization, which allow for direct construction of optically pure compounds from ubiquitous C–H bonds, constitute one of the most central topics in modern organic chemistry. Among different approaches, Co(II)-based metalloradical catalysis emerged out to be a potentially general method for asymmetric C–H alkylation with various of acceptor/acceptor diazo reagents. However, donor-substituted diazo reagents, due to their instability have been much less studied. Herein, we explored Co(II)porphyrin catalyzed asymmetric intramolecular C-H alkylation by using tosylhydrazones as stable equivalence of donor-substituted diazo reagents, affording 2,3-dihydrobenzofuran derivatives in high yields with good enantioselectivity.

GP-22 **Thomas Ghebreghiorgis**[1], Aaron Aponick[1], Daniel H. Ess[2].

[1]Department of Chemistry, University of Florida

[2]Department of Chemistry and Biochemistry, Brigham Young University

Comparative and Mechanistic Studies of Au-Catalyzed Dehydrative Cyclizations of Monoallylic Diols

A comparative study of the gold(I)-catalyzed cyclization of various allylic alcohols and ethers for the formation of tetrahydropyrans (THPs) will be presented. Allylic alohols were found to cyclize faster than allylic ethers. Furthermore, an efficient method to quench Au-catalyzed reaction using scavenging reagent, Reaxa QuadraPureTM MPA, was developed. These results led to extensive experimental and density functional (DFT) investigations on the mechanism and revealed the importance of hydrogen bonding interactions. It was found that the preferred mechanism is a two-step process in which the pendant hydroxyl group attacks the olefin via anti-addition to form a C-O bond followed by anti-elimination of water and the Au(I)-catalyst. Hydrogen bonding plays a great role in templating the stereochemical outcome of this reaction. These results will be presented.

GP-23 **Jennifer Borja**[1], Edward Turos[1].

[1]Department of Chemistry, University of Florida

New Derivates of N-Thiolated B-Lactams: New Dual Action Functionality Impedes MRSA

During one year in our country, MRSA has caused almost 280,000 hospitalizations with a price tag spanning $ 9.7 billion. N-Thiolated B-Lactams inhibit MRSA by stopping Fatty acid biosynthesis, FAB, by scrambling the internal components of MRSA cells while the cell wall remains intact. While lactamases are MRSA's first line of defense against leading antibiotics but they have no effect on N-Thiolated B-Lactams. Making these new dual action drug derivatives a preemptive strike for both drug delivery and drug resistance.

GP-24 **Mona Mohamed[1],** Mike Zaworotko[1].

[1]Department of Chemistry, University of Florida

The mmo Platform: A Family of Highly Versatile Robust Networks for Sleective Carbon Dioxide Capture.

A new class of porous metal organic materials of formula $[M(bp)_2(M'O4]$ (M = Co or Ni; bp = Bipyridine-type linkers; M'O4 = WO_4, MoO_4, CrO_4) has been synthesized based upon saturated metal centres (SMCs) connected by inorganic anions such as WO_4^{2-}, MoO_4^{2-}, or CrO_4^{2-} that affords robust, water and air stable three dimensional porous networks that represent the first examples of 6-c 48.67 topology nets and the symbol mmo was assigned by RCSR. The prototypical mmo structures; CROFOUR-1-Ni, MOOFOUR-1-Ni and WOFOUR-1-Ni were found to exhibit remarkable affinity towards CO_2 gas as exemplified by the exceptional isoteric heats of adsorption (Q_{st}), and high selectivity of CO_2 over CH_4 and N_2. This behavior can be ascribed to the high polarizablity of the inorganic anions which offer favorable electrostatics that can strongly bind with CO_2 bolecules at low pressure regions to outperform MOMs with unsaturated metal centers and tethered amines. These results have been validated by the computational studies which further support the notion of the potential of these MOMs as CO_2 selective adsorbents for applications that are relevant to the post-combustion carbon capture.

The Clear Springs Land Poster Session Abstracts

OR-01 **Vishwajeeth Pasham[1],** Demetrios Pantages[1], Jon Antilla[1].
[1]Department of Chemistry, University of South Florida

Development of an Enantioselective 3,3'-Napthyl Substituted Chiral BINOL-Phosphoric Acid Catalyst

BINOL and BINOL-derivatives have a wide applicability in asymmetric synthesis as chirality inducers. Addition of bulky substituents at the 3,3'-position on the BINOL scaffold have been shown to increase enantioselectivity for certain reactions, such as the asymmetric synthesis of chiral allenes. A scalable procedure for the addition of napthyl substituents at the 3,3'-positions on the (R)-BINOL scaffold is outlined featuring relatively simple workups and providing milligram quantities in moderate yield from commercially available (R)-BINOL. Napthyl addition at the 3,3' position proceeded with a protection step (98% yield), iodination step (52% yield), Suzuki coupling (75% yield), deprotection step (99% yield), and conversion into chiral catalyst via phosphorylation of the BINOL scaffold (50% yield) to yield a total of 500mg of optically pure catalyst from an initial scale of 3.5g of commercially available (R)-BINOL.

OR-02 **Justin Arami[1]**, Benjamin Killian[1], Hong Zhang[1], Zuoquan Wang[1], C. Dennis Hall[1].
[1]Center for Heterocyclic Compounds, University of Florida, Department of Chemistry

Synthesis and Thermodynamic Characterization of Energetic 1,2,4 and 1,3,4-oxadiazoles

Oxadiazoles are a class of five membered heterocycles with diverse chemistry and biological activity that see a wide array of applications including use as bioisosteres, electron transporting materials, and energetic materials. Although energetic materials based on 1,2,5-oxadiazole (furazan) are well known, building blocks based on 1,2,4 and 1,3,4-oxadiazole have received relatively little consideration. In an effort to investigate novel insensitive building blocks for energetic materials, select 3,5-disubstituted 1,2,4- oxadiazoles and 2,5-disubstituted 1,3,4-oxadiazoles were synthesized from commercially available starting material in moderate to good yields and high purity. Combustion analysis was performed by DSC and bomb calorimetry and heats of formation were obtained computationally using semi-empirical and ab initio methods. The oxadiazoles studied showed relatively good combustion performance, high meting points as well as stability during melting, and high positive heats of formation making them possible candidate scaffolds for the further development as insensitive energetic materials.

OR-03 **Erin Mulry[1]**, Olapeju Oyesiku[1], Jianfeng Cai[1].
[1]Department of Chemistry, University of South Florida.

Inhibition of HIV gp41 Fusion with Modified C-peptides

HIV is a worldwide epidemic for which there is currently no cure. Gp41 is an HIV envelope glycoprotein that facilitates interaction between the viral and host cell membranes. After analyzing the known amino acid structure of the C region of gp41, new peptides were synthesized with similar sequences but with some modifications (to enhance stability to hydrolysis) in order to develop a peptide that could inhibit activity of gp41 by blocking interaction between the C and N regions of the protein. Presently, the direct binding studies are in progress. This study tests the binding affinity of the fluorescently labeled C-peptides to the N-peptide through Fluorescent Polarization Assay to obtain the dissociation constant (KD) of the peptides. The goal of this research is to develop a peptide that disrupts interaction of the C region with the N region of gp41, therefore inhibiting injection of viral RNA into the host cell and preventing infection.

OR-04 **Catherine Costa[1,2]**, Ben Eduful[1,2], James Leahy[1,2].
[1]Department of Chemistry, University of South Florida.
[2]Center for Drug Discovery & Innovation, University of South Florida.

Synthesis of a Novel Class of Antileishmaniasis Agents

Leishmaniasis is a disease caused by parasitic protozoa that manifests itself through skin sores that erupt after a host is bitten by sand flies carrying the disease. This presentation reports on the search for molecules that prevent this disease, presumably through the inhibition of the protozoan heat shock protein 90. Hsp90 is a protein that controls both the heat shock response and morphological differentiation and has been implicated in several therapeutic areas. A screening campaign revealed a potential lead compound that has been verified and structural modification to this lead are currently under investigation. We have successfully demonstrated at least the necessity of two methyl substituents on the core ring. The goal is that a compound will be synthesized that is an active hsp90 inhibitor with suitable pharmacological properties and can then be used as a treatment for leishmaniasis.

OR-05 **Allison Mercer[1]**, Haifan Wu[1], Jianfeng Cai[1].
[1]Department of Chemistry, University of South Florida.

Aldol Reaction Catalysis via Synthesized Amphiphilic Peptidomimetics

The goal of this project is to design and synthesize amphiphilic peptidomimetics and test their catalytic activity towards the aldol reaction between cyclohexanone and p-nitrobenzaldehyde in water based solutions. Each of the molecules proposed contains a lipidated hydrophobic core, a catalytic center derived from a γ-AApeptide building block containing a reactive secondary amine, and two glutamic acid residues that serve as a hydrophilic region. The compounds differ in the amino acid derived side chains at the γ position of the catalytic γ-AApeptide building block, being alanine, phenyalanine, or tryptophan. It is hypothesized that these amphiphilic molecules will self-assemble into micelles or nanorods in water and create a hydrophobic and chiral micro-environment that enhances the reaction rate and enantioselectivity of the aldol reaction.

OR-06 **Matthew Jacobsen[1], Elhaam Iranmanesh[1], Ashley Parisi-Goldblatt[1]**, Ali Husain[1], Kirpal S. Bisht[1].
[1]Department of Chemistry, University of South Florida.

Synthesis of Novel Water-Soluble Resorcin[4]arene Cavitand Shielded with Sugar Glucose via Cu(I)-catalyzed Azide-Alkyne Cycloaddition (CuAAC)

Water-soluble resorcin[4]arene was designed and synthesized by coupling polar glucose monomers via multiple 1,4-disubstituted 1,2,3-triazoles in gram quantity. The resulted cavitand composed of a high π-electron rich hydrophobic cavity system surrounded with multiple hydrophilic glucose sugars. The polar sugar parts act as a shield covering the hydrophobic cavity which would act as a cyclodextrin system helping the resorcin[4]arene to be soluble in aqueous medium. The utility of the desired resorcin[4]arene having the advantages containing a cavity which can act as a host-guest molecule and being soluble in aqueous medium may play an important role as a phase transfer catalyst catalyzing organic transformation in water as green chemistry reactions.

OR-07 **Grant Simpson[1,2]**, Khanh Ha[1,2], Alan Katritzky[1,2].
[1]Department of Chemistry, University of Florida.
[2]Center for Heterocyclic Chemistry, University of Florida.
FORUM: Organic_Chemistry

Overcoming the Inherent Difficulty of Peptide Ligation at the Proline Site via Advanced Hydroxyproline Chemoselective Cyclization Methodology

Cyclo-peptides are useful intermediates in drug design. Their application in pharmacuitical and industrial applications, though promising, is limited due to challenging synthesis. Smaller peptides can often be troublesome, if not impossible, to cyclize. Ring size is the most important factor that governs the success of a head-to-tail peptide macrocyclization. In this study, a hydroxyproline-based chemoselective ligation method is proposed, based on known literature proline and Salicyladheyde ester-induced chemoselective peptide ligation at the Serine/Threonine Sites. It uses an O (S)-salicyladehyde ester at the C-terminus, reacting with N-terminal proline to promote peptide ligations. The utilitiy of the S-salicylaldehyde ester enables the rapid coupling reaction and the production of an N,O(S)-benzylidene acetal intermediate, which is readily converted into natural peptidic linkages (Xaa-hydroxyproline) at the ligation site.

OR-08 **Elizabeth Luffman[1]**, Faeez Mahzamani[1], Ashleigh Bachman[1], Kristy Flores[1], Edward Turos[1].
[1]Department of Chemistry, University of South Florida

The Effects of Nanoparticle Chirality on Drug Loading Properties: A Study of Penicillin G-Encapsulated Poly(menthyl acrylate) Nanoparticle Emulsions.

Our laboratory is exploring the synthesis and use of polyacrylate nanoparticle emulsions for antibiotic applications to treat bacterial infections. The main purpose was to determine whether the chirality of a polyacrylate nanoparticle can affect the amount of antibiotic encapsulation. Specifically, we were interested to determine if there exists a correlation between the amount of D-menthyl acrylate contained within a polyacrylate nanoparticle matrix, and the amount of Penicillin G that can be encapsulated inside the particle in aqueous solution. Poly(menthyl acrylate) nanoparticle samples were prepared and loaded with Penicillin G at concentrations ranging from 0%-20% by weight. For each sample emulsion, we used dynamic light scattering to measure the zeta potential and diameter of the nanoparticles obtained, and optical polarimetry to determine the optical rotation values. These data enabled us to begin assessing, for the first time, the influence of a nanoparticle's chirality on antibiotic encapsulation for possible drug delivery applications.

OR-09 **Vidya Hanuman[1]**, Yi Liang[1], Anthony Gebhard[4], Rajesh Nair[2,3], Lori Hazelhurst[2,4], Mark L. McLaughlin[1,2, 3].
[1]Department of Chemistry, University of South Florida.
[2]Modulation Therapeutics.
[3]Drug Discovery H. Lee Moffitt Cancer Center.
[4]Molecular Oncology, H. Lee Moffitt Cancer Center.

Exploring the Use of MTI-101 in the Human Body via Synthesis of β-turn Promoters

Multiple Myeloma (MM) poses a serious threat to the overall health of elderly individuals. It causes increased levels of plasma in bone marrow and leads to the production of atypical proteins in the bloodstream. To counteract these effects, cyclic peptide MTI-101 was developed to promote necrosis of MM tumor cells. The aim of this research project involves synthesis of β-turn promoters which are attached to biological molecules that work to improve the bioactivity and understand how MTI-101 cures MM. The synthesis of the linker D-prolinol and other linker derivatives occur via SN2 reactions. Through this method, it is expected that the various functional groups which

attach to the peptide, extends the in vivo circulating half-life of MTI-101. For future experiments, side chains of various linkers with differing functional groups can be modified and combined with other biological molecules to determine their effects on the bioactivity of MTI-101 in vivo.

OR-10 **Andrea Lemus**[1], James W. Leahy[1].
[1]Department of Chemistry, University of South Florida

Novel Synthesis of (+)-Catechin Metabolites

Catechin is a compound present in most plants and is metabolized into smaller molecules by the liver when ingested. The function of these metabolites is unknown, although this class of molecules has been shown to have anti-inflammatory properties and therefore could be useful in the areas of diabetes and heart disease research. It is also unknown if catechin metabolites are targeting a particular enzyme. We wish to report our efforts to synthesize 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 study of the effects of these compounds in the body can lead to potential new therapies for diabetes.

OR-11 **Kristy Flores**[1], Faeez Mahzamani[1], Ashleigh Bachman[1], Elizabeth Luffman[1], Edward Turos[1].
[1]Department of Chemistry, University of South Florida

A Study on the Stability and Uniformity of Enantiomerically-Pure Penicillin-Encapsulated Poly(menthyl acrylate) Nanoparticle Emulsions

While the β-lactam antibiotics have proven to be incredibly effective at inhibiting microbial growth, certain pathogenic bacteria such as methicillin-resistant Staphylococcus aureus (MRSA) have developed antibiotic resistance. In an effort to increase the efficacy of β-lactam antibiotics, our laboratory has begun to explore alternative ways to enhance their efficacy against MRSA using polyacrylate nanoparticle delivery vehicles. In the current study, we examine new emulsified nanoparticles prepared from enantiomerically-pure D- and L-menthyl acrylates by radical-initiated emulsion polymerization, in the presence of different quantities of penicillin G. Dynamic light scattering (DLS) was used to measure the size and the stability of the nanoparticle samples. These results indicate that the emulsified penicillin-encapsulated nanoparticles are highly uniform in size and stability at all drug concentrations examined, suggesting their potential use in antibiotic drug delivery.

OR-12 **Piero Carletti Bonomo**[1], Ankush Kanwar[1], James W. Leahy[1].
[1]Department of Chemistry, University of South Florida.

Studies Aimed at the Synthesis of N-Linked Hsp90 Inhibitors as Antileishmaniasis Agents

Leishmaniasis is a parasitic disease transmitted by the bite of sandflies. There are two primary types of leishmaniasis, cutaneous and visceral. Visceral leishmaniasis is typically lethal if not treated promptly and properly. Since the traditional treatments for cutaneous leishmaniasis, antimony and amphotericin, are not very effective against visceral leishmaniasis, alternative treatments are of paramount importance. In a screening campaign by Professor Dennis Kyle, a novel chemotype was revealed to be active against Leishmania donovani amastigotes that had previously been demonstrated to inhibit the chaperone protein Hsp90. In a collaborative effort, we are designing and synthesizing novel analogs of this initial hit aimed at improving the activity as well as the ADME and pharmacokinetic characteristics with the hopes of discovering a potential drug candidate for the treatment of this disease.

OR-13 **Sadra Hamedzadeh**[1], Khanh Ha[1], Alan R. Katritzky[1].
[1]Department of Chemistry, University of Florida.

Peptide Cyclodimerization by Pd-Mediated Deprotection Lactamization

Cyclic tetrapeptides are very rigid medium-ring structures. Different conformers of these molecules have been isolated, and these have been shown to display different biological activities. Although isolation and structure determination of these compounds have taken place over the past three decades, there has been little success in synthesizing representative compounds due to ineffective cyclization of a linear tetrapeptide. Bringing the two termini sufficiently close to induce cyclization in such small molecules is challenging, and virtually impossible with the currently used synthetic methods. Utilizing a Pd-assisted tandem deprotection-cyclization reaction, we selectively convert open-chain N-Cbz-dipeptidoylbenzotriazolides to form both symmetric and asymmetric cyclic tetrapeptides. This methodology was successfully demonstrated by ring-closure of a series of dipeptidoylbenzotriazolides yielding cyclo-tetrapeptides, which cannot be prepared efficiently using previously reported methods. The approach described here should provide a convenient entry for the design of a variety of cyclo-tetrapeptides with potential utility in medicine, catalysis, and material science.

OR-14 **Lucas W. Hernandez**[1], Susana S. Lopez[1], Jon C. Antilla[1].
[1]Department of Chemistry, University of South Florida.

Enantioselective Brønsted Acid-Catalyzed Hydroboration of α,β-Unsaturated Ketones

The synthetic strategy of enantioselectively reducing carbon-carbon double bonds is a well-recognized and powerful tool in an organic chemist's arsenal. Many organocatalytic methodologies have been developed which chemo- and enantioselectively reduce α,β-unsaturated ketones. Although these methodologies were successful in cyclic systems, linear systems did not yield the same results and usually incorporated toxic metals. The methodology developed here avoids the use of metals, integrating an organic chiral phosphoric acid catalyst instead, and successfully reduces the linear α,β-unsaturated ketones with excellent conversion and enantioselectivity.

OR-15 **Lamont Nash**[1], Arthur Maknenko[1], Kirpal Bisht[1].
[1]Department of Chemistry, University of South Florida.

Opening of Lactones to Yield Hydroxy Esters

A caprolactone was subjected to a ring opening to yield its respective acyclic hydroxy ester. The reaction proceeded via the refluxing of the ε-caprolactone with sodium methoxide in methanol. Once the reaction was shown to be complete via TLC, the methanol was removed resulting in the pure acyclic product. The percent yield was then able to be calculated. The same procedures were taken to open the 15-lactone. However, unlike the ε-caprolactone, which is a liquid at room temperature, the 15-lactone is a solid therefore it had to first be dissolved in methanol. Nonetheless, both were shown to be very efficient and quantitative reactions.

OR-16 **Anthony Peters**[1], Tamalia Julien[1], Julie P. Harmon[1].
[1]Department of Chemistry, University of South Florida.

An Investigation of the Self-healing and Recovery Properties of Carbon Black-Polycarbonate Polyurethane

The purpose of this study is to investigate the effect of carbon black on the self-healing and recovery properties of polycarbonate polyurethane (PCPU). This research is important because it will provide insight into new materials that have possible applications in various industries, particularly in biomedical industry. Due to PCPU's self-healing

and recovery it has potential for a variety of applications in the biomedical industry ranging from uses as diverse as skin grafts to cardiac bypasses.
It is hypothesized that hydrogen bonding is responsible for these exquisite properties of the polymer. In this experiment four different polymers were made. One of these polymers was a PCPU + dichloromethane control, and the other 3 were polymers of PCPU + dichloromethane + carbon black at 0.5%, 0.75%, and 1.0 % concentrations. Fourier transform infrared spectroscopy (FTIR) was used to investigate if hydrogen bonding causes the self-haling and recovery properties.

OR-17 **Jaime Ibanez**[1], Tamalia Julien[1], Julie P. Harmon[1].
[1]Department of Chemistry, University of South Florida.

Improving the Recovery Time, Mechanical Properties and Toughness of Self Healing Poly Carbonate Poly Urethane Polymers with Silica filler.

This research aims to improve the characteristics of a polymer that can self heal by adding different concentrations of Silica filler. This polymer is made up of Poly carbonate poly urethane (PCPU) and it self heals via inter-diffusion and hydrogen bonding. The characteristics that my lab intends to improve are its recovery time, mechanical properties and toughness.
Previous studies have shown that nanotubes can improve the characteristics of PCPU that we aim to improve. Nevertheless, these nanotubes are too expensive so my lab intends to find a substitute that can give similar properties to PCPU polymers. These substitutes will be dissolved in a PCPU/ DCM (dichlormethane) solution by sonicating the mixture. If the substitutes improve, the polymer this will allow the production of low cost synthetic cartilages and peacemaker wires that can self heal.

OR-18 **Ian Childers**[1], Sri Nimmagadda[1], Jon Antilla[1].
[1]Department of Chemistry, University of South Florida.

Asymmetric Mukaiyama-Michael addition of Silyl Ketene acetal to β-nitrostyrene

Mukaiyama Michael addition reaction of enolsilanes with α,β-unsaturated carbonyl compounds catalyzed by Lewis acid is well known and several asymmetric variants of this reaction have also been reported in literature. The Michael addition of silyl ketene acetals to nitrostyrenes forms γ-nitro carboxylic acid derivatives which could be converted to γ-aminoacids. We are developing the asymmetric Mukaiyama Michael addition reaction to nitrostyrene by using chiral BINOL Phosphoric acid and chiral BINOL Phosphate metal complex as catalysts.

OR-19 **Ali Siddiqui**[1], James Leahy[1].
[1]Department of Chemistry, University of South Florida.

Synthesis and optimization of a novel drug candidate that exhibits promising antibacterial bioactivity against antibiotic resistant pathogens

The alarming development of antibiotic resistance by various pathogenic bacteria poses an immediate and substantial danger. Resistant bacterial strains have the potential to instigate unhindered epidemics because current treatment methods have largely been rendered ineffective against these novel pathogens. Methicillin-resistant Staphylococcus aureus (MRSA) and Vancomycin-resistant Enterococcus (VRE) are antibiotic resistant pathogens that have proliferated due to the absence of effective antibiotic treatments. Membranolide-A is a natural product isolated from the Antarctic sea sponge Dendrilla membranosa that belongs to a class of compounds with established antibacterial bioactivity against resistant pathogens, including MRSA and VRE. This study aims to elucidate the absolute stereochemistry of membranolide-A via total synthesis and to optimize the bioactivity of membranolide-A through production of synthetic analogs. Production of a novel antibiotic with therapeutic efficacy

against resistant pathogens is of utmost pertinence in order to avert impending epidemics that could result from the continued propagation of antibiotic resistant bacteria.

OR-20 **Ashleigh Bachman**[1], Faeez Mahzamani[1], Kristy Flores[1], Elizabeth Luffman[1], Edward Turos[1].
[1]Department of Chemistry, University of South Florida.

Synthesis and Characterization of Novel Penicillin G-loaded Chiral Nanoparticles for Drug Delivery Applications

Our laboratory is exploring the synthesis and use of polyacrylate nanoparticle emulsions for antibiotic applications to treat bacterial infections. The purpose of this research project was to examine poly(menthyl acrylate) nanoparticles as carriers of antibiotics, to try to circumvent the ever-growing antibiotic resistance of deadly Staphylococcus aureus bacteria. To do this, we used the D- and L-stereochemical forms of menthyl acrylate as monomers to synthesize chiral nanoparticles as an aqueous emulsion. This was achieved via acrylation of enantio-pure D- and L-menthol, with subsequent radical polymerization in the presence of sodium dodecyl sulfate (SDS) as a surfactant. The emulsion polymerization was done in the presence versus the absence of a model antibiotic (penicillin G), with final drug load amounts from 0- 20% by weight. The relative stability and size of each nanoparticle sample was then determined by dynamic light scattering to assess the effect of nanoparticle chirality on antibiotic drug loading.

OR-21 **Margarita Vanegas[1], Oleg Tsvyetayev[1],** James Leahy[1].
[1]Department of Chemistry, University of South Florida.

Synthesis of Xanthurenic Acid Analogues

Infectious diseases are the leading cause of death among children as well as the second leading cause of all human death worldwide. In 2010, there were estimated 200 million cases and 660,000 deaths due to malaria, one of the most dangerous infectious diseases. The parasitic source of malaria are Apicomplexa of the genus Plasmodium, which have a complex life cycle. Human infection occurs through sporozoites, which move into liver to mature into merozoites and infect red blood cells. Some of these merozoites mature further into gametocytes, which do not mature further in the human host. 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 thus to lower the incidence of malaria.

AN-01 **Michael Pare[1]**, Michael Doligalski[1,2], Mohanraja Kumar[1,2].
[1]Department of Chemistry, University of South Florida
[2]University of South Florida Mass Spectrometry/Peptide Facility

Developing Methods for the Purification and Characterization of Amyloid-β peptides using HPLC, LCMS, and Circular Dichroism Instruments

Various analytical instruments can be employed for use in a laboratory to elucidate the chemical and physical properties of compounds that are being studied, and to purify them for greater use in research experiments. This presentation focuses on the use of HPLC, LCMS, and Circular Dichroism instruments to elucidate the physiochemical properties of two fragments of the Amyloid Beta peptide that is a key element in the pathology of Alzheimer's disease. Optimized methods were developed to obtain the highest resolution and signal strength of peptide analytes on each instrument. Findings suggest that the degree of nonpolarity varies between different fragments of the peptide, and that protein folding patterns will vary depending on its primary structure. Findings from this study demonstrate how researchers can adopt more effective strategies for developing methods using these instruments in their studies, while conserving time and resources in the process.

AN-02 **Hilary Brown[1]**, Jennifer Speer[1], John Gerling[2], Kenyon Evans-Nguyen[1].
[1]Department of Chemistry, Biochemistry, and Physics, University of Tampa.
[2]Gerling Applied Engineering.

A Mass Spectrometer for Elemental Analysis based on Fieldable Technologies

Laser ablation (LA) can facilitate direct analysis of solid samples for mass spectrometry (MS), and is often coupled with an inductively coupled plasma torch (ICP). LA-ICP-MS is now widely used for accurate elemental and isotopic analysis; however, the technique is not fieldable, primarily due to the gas and power requirements of the ICP torch. A mass spectrometer system for elemental and isotopic analysis using technology that is amenable to portable instrumentation is being studied. Solid samples are being ablated with an excimer laser and the resulting particle and ion plume will flow through a microwave plasma torch (MPT) and into an ion trap mass spectrometer. Preliminary data confirms that using laser ablation directly coupled with an ion trap mass spectrometer is a viable technique for detecting metals (e.g., lead, cobalt) and refractory compounds (e.g., strontium titanate). Current efforts are focused on enhancing sensitivity by incorporating a custom MPT. MPTs, laser ablation and ion trap mass spectrometers can all be incorporated into portable instruments.

AN-03 **Kayleigh Farnham[1]**, Garrett Craft[1], Tamalia Julien[1], Kenneth Kull[2], Alejandro Rivera[1], J. Harmon[1].
[1]Department of Chemistry, University of South Florida
[2]Solicore, Inc.

Analysis of Hydrogen Bonding Among Polyimides Using FTIR -ATR

Fourier Transform Infrared (FTIR) Attenuated Total Reflectance (ATR) is a spectroscopic technique used to analyze various compounds and their infrared active components. This technique will be employed in the analysis of the hydrogen bonding of polyimides (PIs), with no difference except their elongated repeating units, to determine which regions of the molecule will be affected by this phenomenon. Analyzing the compounds as powders, films, and molds allows for variations in the amount of solvent and/or concentration of the (PIs) to be taken into consideration for the compounds. There are five different compounds and films all were dissolved in n-methyl-2-pyrrolidone (NMP).

AN-04 **Rebeca Pupo[1]**, Abdullah Alhendal[1], Abdul Malik[1].
[1]Department of Chemistry, University of South Florida

Gas Chromatographic Analysis of the Progression of the Maillard Reaction in Milk Caramel using Capillary Microextration

This experiment aims to examine the progression of the Maillard reaction in milk caramel (using sucrose reduced to fructose and glucose reacted with amino acids from fat-free milk) using sol-gel capillary microextraction (CME). The sorbent on the inner surface of the capillary to act as the extraction phase. After coating, the capillary was tested with various chemicals similar to the chemicals produced in the Maillard reaction to ensure sharp peaks can be obtained. Then the milk caramel was cooked and samples were taken at various points in the cooking process, used in extraction with the CME, and then examined in the gas chromatograph. There are obvious changes in the chromatograms as the samples are cooked based on the chromatograms. indicating that this sol-gel recipe can be used successfully to examine the progression of the Maillard reaction in milk caramel.

IN-01 **Ilia Toli[1],** Pedro Patino[1].
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Data Storage on Single-Layer Fluorographene Sheets

A data storage chip made of a single layer Fg (fluorographene) sheet is proposed. It stores 0.5 PB/cm2 data. This is 500,000 GB/cm^2. In stand alone it is tear resistant and stable for up to 24 hours in temperatures up to 400°C. On a support surface at room temperature it is stable indefinitely. Various methods for writing and reading are proposed. The Fg sheet may be placed on a support surface, typically a single-crystal silicon sheet. The support and the Fg sheet can be stacked up in 3D. This dramatically increases the density of information storage. No stereochemical rearrangements are expected to occur because of the tight arrangements of carbon in graphene. Stereochemical deformations should be minimal, local and not problematic, furthermore minimized by the van der Waals forces of the support sheet. The Fg sheet is kept firm into place on all of its borders.

IN-02 **Kevin Mulles[1]**, Chavis Stackhouse[1], Shengqian Ma[1].
[1]Department of Chemistry, University of South Florida.

Porous Metal Organic Frameworks - Organized Porous Structures with Atomic Precision

Covalent porous crystalline polymers incorporate organic building blocks into organized structures leading to new potential applications of methods such as gas storage, CO_2 capture, solar energy and much more. These atomically structured polymers are difficult to synthesize but are being researched thoroughly for their desirable low mass density, high thermal stability and permanent porosity. In order to form a flexible macrocycle with coordination diversity and substantial CO_2 uptake, tactmb, an azamacrocyclic tetracarboxylate ligand, was synthesized and reacted with $Cd(NO_3)_2 \cdot 4H_2O$ in N,N-dimethylformamide for 48 hours. The product resulted in a 3-D colorless block crystal of Metal-Macrocyclic Framework. This framework was successful in providing permanent porosity and selective uptake of CO_2 over N_2. Possible grafting of primary, secondary or tertiary amine groups into porous metal organic frameworks (MOF) may significantly increase the uptake of CO2 in the synthesis of future MOF's.

IN-03 **Christopher McKeithan[1],** Christian Tang[1], Li-June Ming[1].
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Spectroscopic Investigation of Sugar Groups of Flavonoids on Metal Binding Affinity

Flavonoids are naturally occurring secondary metabolites found in most plants. They possess significant potential for research into their many beneficial qualities i.e. antioxidant, neural protection. Four flavonoids, Rutin, 5-hydroxyflavone, Hesperetin, Hesperidin, were chosen for spectroscopic investigation. Two of these flavonoids have sugar substitutions (Rutin and Hesperidin). The effect of this substitutes is the primary purpose of investigation. Binding affinity of each flavonoid will first be determined using Cu2+ in each of the available solvents. The flavonoids will then be kinetically studied in a system of 3,5-ditert-butylbenzene-1,2-diol (DTBC), copper beta-amyloid (Cu-Aβ), and HEPES buffer. The DNA cleavage of each flavonoid will be determined using gel electrophoresis. The conclusion will be based on the catalytic activity based on interaction with each of the four flavonoids.

IN-04 **Sy-woei Hao[1], Thu Suong Le[1]**, Christian Tang[1], Li-June Ming[1].
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tert-Butylcatechol Oxidation Chemistry of Fragments of Alzheimer's Disease-related β-Amyloid Peptide

Gradual and rapidly created illnesses found in the human body leads to the development of discovering cures and other preventatives. The purpose of this experiment is to identify the association between fragments of the Alzheimer's disease-related beta-amyloid peptide (CuAβ) and oxidation to seek reduction of symptoms in Alzheimer patients. By running an inhibition reaction, the concentration of ferulic acid was increased to determine the change in oxidation rates. Using the Hanes kinetic method, the value of competitive inhibition will be analyzed between the substrate and ferulic acid. In this ongoing experiment, increasing the concentration of ferulic acid is predicted to decrease the oxidation rate. Further analysis will take place using gel electrophoresis to observe the presence of DNA cleavage. However, if experimental values do not illustrate a significant inhibition by varying ferulic acid, the introduction of caffeic acid acting as a substrate will be a substitution used to determine correlation.

The Solomon T. Weldegirma Poster Session Abstracts

BC-01 **Luis R. Saavedra Román[1]**, Robert Sprung[1], Mark Meads[1], Ian Pike[2], Ken Shain[2], John Koomen[1].
[1]H. Lee Moffitt Cancer Center, Tampa, FL
[2]Proteome Sciences, London, UK

Multiplexed Detection of Apoptotic Proteins using Peptide-Based Separations

Apoptosis proteins are critical for cancer treatment due to their key role in cell death; therefore, assessment of apoptotic protein expression is a key to developing the best treatments. Currently, determination of the best treatment focuses on different doses and combinations of therapeutic agents, so the measurement needs to be high throughput. The standard method uses SDS-PAGE to separate the apoptotic proteins, which all have a low molecular weight. This technique is labor intensive and hard to apply to a large amount of samples. Peptide isoelectric focusing(IEF) and basic pH reversed phase chromatography(bRPLC) are explored as alternative methods to allow for more flexibility, greater compatibility with other multiplexed proteomics approaches, and the ability to analyze archived patient specimens. Peptide-based methods are then compared to protein-based methods as a standard to confirm that they give the same results. This study can aid researchers in determining combination therapies for cancer.

BC-02 **Anne-Marie Carpenter[1]**, Daniel Dempsey[1], Santiago Rodriguez Ospina[1], David Merkler[1].
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Mechanistic and Structural Analysis of Drosophila Melanogaster Arylalkylamine N acetyltransferase Like 7

Histamine is a biogenic amine that regulates several neurological processes in Drosophila melanogaster. A catabolite of this neurotransmitter known as N- acetylhistamine has been found in the Drosophila head. Herein, we show that N-acetylhistamine and other N-acetylated biogenic amines are formed by an enzyme known as arylalkylamine N-acetyltransferase like 7 (AANATL7), which catalyzes acetyl-coenzyme A-dependent N-acetylation of histamine and arylalkylamine substrates. We used double reciprocal analysis and dead-end inhibition to define the kinetic mechanism for AANATL7. The kcat,app pH rate profiles revealed apparent pKa values of catalytic residues that suggested a chemical mechanism involving acid/base catalysis. Site directed mutagenesis of catalytic residues supported the acid/base chemical mechanism. Several amino acids were also implicated as structurally important in substrate binding and product release. These data further clarify the role of AANATL7 in the neurological functioning of Drosophila melanogaster.

BC-03 **Santiago Rodriguez-Ospina[1]**, Daniel R. Dempsey[1], Anne-Marie Carpenter[1], David J. Merkler[1].
[1]Department of Chemistry, University of South Florida.

Mechanistic and Structural Analysis of Drosophila Melanogaster Polyamine N-acyltransferase

Fatty acid amides consist of short and long-chain N-acylethanolamines, N-acyl amino acids, N-arylalkylamides, and the N-monoacylpolyamides. These metabolites are an emerging family of lipids involved in the inactivation of neurotransmitters, as cell signaling lipids, insect cuticle sclerotization, and in the biosynthesis of melatonin. Polyamines has been shown to have antinociceptive, anticonvulsant, and anti-depressant bioactivity, while diseases including cancer and Snyder-Robinson syndrome have been attributed to dysregulation of polyamine biosynthesis.
One biosynthetic step in the catabolism of the polyamines is the enzyme-catalyzed formation of N-monoacylpolyamines, which is catalyzed by a polyamine N-acyltransferase (PNAT). PNAT from D. melanogaster is a member of the Gcn5 related N-acetyltransferases family which catalyzes the N-acylation of polyamines from the corresponding acyl-CoA. Herein, we report the evaluation of structure-function relationships and data suggesting a chemical mechanism for enzyme-catalyzed formation of N-monoacylpolyamines for D. melanogaster PNAT.

BC-04 **Tatyana Gurina[1], Imran Gruhonjic[1]**, Kristen A. Jeffries[1], David J. Merkler[1].
[1]Department of Chemistry, University of South Florida.

Heavy-labeled Precursor Feeding Studies Give Insight to the Biosynthesis of Long-chain Fatty Acid Amides in Neuroblastoma Cells

Fatty acid amides (FAAs) are endogenous signaling lipids that have various biological functions in mammals. Although the biosynthetic pathways of long-chain FAAs are not completely understood, data about their metabolism could lead to novel therapeutics. We have identified and quantified the endogenous levels of long-chain N-acylglycines, N-acyldopamines, N-acylethanolamines, and primary fatty acid amides in N18TG2 nueroblastoma cells. The N18TG2 cells were fed heavy labeled 13C-palmitate and incubated, yielding unlabeled and labeled long-chain FAAs. The FAAs were extracted from the cells, purified, analyzed by LC-QTOF-MS, and quantified using standard curves. The 13C-palmitoylated fatty acid amides that were identified support the biosynthetic pathways of long-chain FAAs proposed herein. Since these molecules are being produced in N18TG2 cells, the cells must also express the enzymatic machinery needed to make them. Ongoing experiments include quantifying FAAs from N18TG2 cells after siRNA knockdown of the enzymes proposed to be involved in their biosynthesis.

BC-05 **Toral Shah[1], Saman Shamsi[1],** Yao Chen[1], Shengqian Ma[1].
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Catalysis Reactions

Introduction: In the many experiments performed in this lab, some key points that are being tested on is the absorbency of cytochrome C and how fast a reaction would act with a certain chemical acting as a catalyst, such as peroxide. The aim is to find the rate and absorbency of cytochrome C under different circumstances.
Methods: A cuvette containing different amounts of cytochrome C, peroxide, HEPES buffer, and THB is put into a spectrometer to calculate the rate of reaction and absorbency.
Results: The more THB that is used slows the rate of reaction.
Conclusion: The concentration of the substrate does affect the rate of reaction. When conducting similar experiments, other substances such as TB Mof crystals are added in cytochrome C to see if that affects the rate or absorbency of the reaction. The substrate is entitled to change as well.

BC-06 **Lucia Franco Estrada[1]**, Tamalia C. M. Julien[1], Julie Harmon[1].
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Investigating Differences in Healing Properties between Neat PCPU, PCPU + Carbon Black, and PCPU + Nano Silver

Polycarbonate Polyurethane (PCPU) is an autonomic self-healing material that does not require external triggers to heal. The aims of this study were to investigate the difference in absorbance peaks, tensile strength, and thermal properties between neat PCPU, PCPU+carbon black, and PCPU+nano silver. Nanocomposite samples different in % by weight were made: 5 carbon black samples (0.25- 2%) and 4 nano silver samples (0.1-2%). FTIR was used to obtain the absorbance peaks of uncut and cut samples, the tensile tests were manually performed, and the thermal properties were measured with a DSC. For the nanocomposite samples the absorbance peaks, the time needed to break the different samples, and the thermal properties were greater than the corresponding values for neat PCPU. Thus, the added nanocomposites enhanced the healing properties of neat PCPU. Since this is an ongoing research more experiments should be performed to verify the results obtained in this study.

PC-01 **Selamawi Ambaye[1],** David Rogers[1].
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Computation of the Spatial Diffusion Coefficients and Diffusive Flux of Methanol in Water Using Molecular Dynamics Simulations

Having a predictive model for the diffusion process is important because diffusion is involved in a variety of chemical and biological systems including the diffusion of particles through a membrane,diffusion of proteins, as well as several other industrial processes that involve diffusion. The main goal of this paper is to compute the spatial diffusion coefficients and diffusive flux of methanol in water using the equation J(P) = C [P], where J represents a flux density P represents a number density and C is a constant that contains the spatial diffusion coefficients. The equation J(P) = C [P] assumes that the flux J(molecules/m^(2)s) is a function of number density P which means that instead of attributing the diffusion process to a concentration gradient, this equation states that molecules move from one position to another because they are influenced by neighboring molecules.

PC-02 **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 does so by rapidly increasing the concentration of bioavailable nitric oxide (NO). Heme enzymes in the blood, including catalase, are most likely responsible for the release NO. It is our goal to use a suite of computational methods to predict the most likely reaction pathway for the release of NO by catalase and to propose more efficient NO releasing substrates. A catalase compound I structure has been prepared using CHARMM force fields and MD simulations and QM/MM methods have been used to generate optimized active site geometries for doublet, quartet, sextet, and octet spin states. Binding mode analysis of PubChem has been done to identify other possible NO releasing substrates. We have identified that non-polar R-group on the opposite side of the hydroxylamine, should allow favorable interaction for proper orientation over the heme during reaction.

PC-03 **Jacob Wilson**[1], Sreya Mukherjee[1], Wesley Brooks[1], Wayne Guida[1].
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Drug Discovery in SAM Decarboxylase Using Virtual Screening

The polyamines (putrescine, spermidine and spermine) are essential for many functions in the cell. For example, they are required for cell replication, transcription of genes and protein expression. However, when polyamines are at abnormally high levels, they can interfere with normal cellular activities and possibly initiate diseases. S-adenosylmethionine decarboxylase (SAMDC) is an enzyme which plays a key role in the biosynthesis of spermidine and spermine. However, SAMDC competes for the molecule SAM which is also used in DNA methylation, i.e. gene silencing. If SAMDC is over-active, then other genes can become overly active as they escape gene silencing, such as in some cancers and autoimmune diseases. Therefore, SAMDC is a potential therapeutic target to treat these diseases. Herein, we look into inhibition of SAMDC via virtual screening with small molecules of the NCI diversity set. These inhibitors may eventually be used in the treatment of diseases.

PC-04 **Tyler Waid**[1], Sreya Mukherjee[1], Sreya Mukherjee[1], Wayne Guida[1].
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Structure Modification of Apolipoprotein E4 to Restore Normal Functionality

Alzheimer disease is the most common form of dementia. Its pathogenesis incorporates many potential targets for treatment. Among the targets identified, Apolipoprotein E4 (apoE4) is especially interesting due to its catalytic role in the degradation and clearance of amyloid beta (Aβ), a risk factor for Alzheimer disease. ApoE exists in 3 isoforms which directly impact its functionality in the body. There are characteristic structural differences between them. In ApoE4 ionic interactions exist between Arg-61 and Glu-255 residues, unlike the other isoforms. Hence interruption of this interaction by small molecular inhibitors may change the structure of apoE4 to a more linear structure as observed in the other isoforms. Virtual screening of the NCI diversity set on an energy minimized protein virtual structure was performed to identify potential small molecule inhibitors and to gain further understanding of interactions that can be targeted to inhibit this protein.

PC-05 **Shane Burger**[1], Sreya Mukherjee[1], Wesley Brooks[1], Wayne Guida[1].
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Drug Discovery of N1-acetlytransferase- an Enzyme in the Polyamine Synthesis Pathway Using Virtual Screening

Polyamines serve many functions in the body. Many of these functions are thought to be regulatory, such as stabilization of large macromolecular complexes of proteins and DNA. However, polyamine synthesis competes with methylation and suppression of genes since both polyamine synthesis and cellular methylation use the molecule, S-adenosylmethionine (SAM). To stabilize polyamine levels, polyamines can be synthesized by spermidine synthase and spermine synthase and recycled by spermidine/spermine N1-acetlytransferase (SSAT1). Overexpression of polyamine enzymes could lead to continual synthesis and recycling, wasting SAM and disrupting methylation needed for gene suppression, potentially leading to disease states. Inhibition of SSAT1 would break this futile cycling through the polyamine pathway. Therefore, we are performing virtual screening with small molecules, such as the NCI diversity set, against a virtual structure of SSAT1 to identify potential inhibitors as an initial step in drug discovery and development.

PC-06 **Carlie Craven[1]**, Sreya Mukherjee[1], Wesley Brooks[1], Wayne Guida[1].
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Drug Discovery of Spermine Synthase Using Virtual Screening

Polyamines are ubiquitous molecules that have important interactions with nucleic acids, phospholipids, and proteins. Polyamines are essential for cell growth, differentiation and other functions. Disruption of polyamine levels is believed to play a role in diseases; from cancers to autoimmune diseases, like rheumatoid arthritis. Mammals produce three polyamines; putrescine, spermidine and spermine. The polyamine pathway uses aminopropyl groups derived from S-adenosylmethionine (SAM) in the production of spermidine and spermine. This process is highly regulated in cells since SAM is also used in cellular methylation to suppress genes. Over activity of polyamine synthesis could lead to reduced SAM levels and loss of gene suppression, which may have a role in diseases. We are targeting the enzyme spermine synthase (SMS) in virtual screening as an initial step in identifying small molecules that inhibit SMS and which could be developed into drugs.

PC-07 **Mariafernanda Davila[1]**, Sreya Mukherjee[1], Wesley Brooks[1], Wayne Guida[1].
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Computational Study of 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 ketones was constructed and screened against a virtual structure of 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.

PC-08 **Linh Le[1], Fatmaelzahraa Abdelmola[2]**, Manoj K Ram[1], Yogi Goswami[1], Ashok Kumar[2], Elias Stafanakos[3].
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Photoelectrochemical Hybrid Nanofilm

The photoelectrochemical cell has been found to be attractive due to conversion of optical to electrical energy, sensor and water splitting applications. The photoconversion efficiency of photochemical cell is nearly par with metal oxide based photovoltaic device. Our group is active in studying the photoelectrochemical properties of poly(methylthiophene), poly(octylthiophene), ragioregular polyhexylthiophene (RRPHTh) and several substituted polythiophenes in nanohybrid structure using nanodiamond, ZnO and TiO2 nanomaterials in conducting polymer matrix. The recent photoelectrochemical studies have shown 8 to 10 times of photocurrent enhancement in RRPHTh-nanodiamond (ND) hybrid film in close comparison to ZnO- RRPHTh and TiO2- RRPHTh hybrid films. This manuscript finds the experimental finding of photoelectrochemical properties of ND-polyaniline (PANI) hybrid films. Besides, the molybdenum disulfide (MoS2)–RRPHTh hybrid structures have been extensively characterized. The photoelectrochemical study has shown that RRPHTh acted as an electron donor and MoS2 as electron acceptor in MoS2 –RRPHTh nanostructure film. The MoS2 –RRPHTh has been found to be interesting nanohybrid structure for future exploitation of photoelectrochemical cell.

PC-09 **Phillip Hudson[1],** Gerhard Koneg[2], Stefan Boresch[3], H. Lee Woodcock[1].
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Non-Boltzmann Bennett Reweight: A Novel Approach to ensure Relevant Sampling in Free Energy Simulation

Free energy simulation (FES) is a sampling based approach to free energy calculations. Considered a standout FES method; Bennett's acceptance ratio (BAR) is an efficient method used to compute free energy change between two super states with distinct potential energies. QM/MM modeling in conjunction with FES via BAR reweighted scheme results in the contribution of each frame scaled by how well the QM and MM energies agree. This scheme named the non-Boltzmann Bennett (NBB) method allows for confident sampling by eliminating non-contributing states. Using this newly developed method, hydration free energies were calculated for a set of 21 biochemically significant molecules in MM implicit solvent models. Test set results for NBB showed a root mean square deviation (RMSD) of 0.76 kcal/mol, which shows improvement compared to standard BAR method (RMSD 1.79 kcal/mol). The NBB method improves free energy calculation accuracy and shows promise for novel systems of interest.

NP-01 **Mfonobong Inyang[1]**, Danielle H. Demers[1], Bill J. Baker[1, 2].
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The Optimization of Fungal Culture Techniques for a Drug Discovery Screening Project

Natural products play a huge role in the development of drugs against human diseases. Approximately 2/3 of all new chemical entities approved between 1981 and 2006 are natural products or their derivatives. Fungi are a great source of bioactive secondary metabolites. In the Baker Lab, fungi are subjected to a culturing process that includes epigenetic modification. Epigenetic modification activates the gene clusters that may be down regulated or silenced in normal laboratory conditions. This is done with the addition of small molecule modifiers to the culture medium. The current method being used in the fungal screening project, though successful, has never been fully optimized. The purpose of this culture optimization study is to reduce contamination, and get the highest possible extract mass, metabolite diversity and bioactivity.

NP-02 **Keith Zimmerman[1]**, Ryan Young[1], Laurent Calcul[1,2], Bill J. Baker[1,2].
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Use of High-Throughput Screening to Identify Potential Anti-Plasmodials.

The malaria parasite Plasmodium sp. kills approximately 2,000-3,000 people per day and resistance to the once widely used drug chloroquine has spread to most areas affected with the disease, so new drugs are required to overcome this resistance. The metabolism of hemoglobin by the malaria parasite, Plasmodium sp. releases heme, which is toxic to the parasite. This toxicity is overcome by the crystallization of heme to hemozoin. This is not an enzyme mediated process, and resistance is caused by a process of pumping the drug out by membrane proteins rather than modification of the active site, so is an ideal target for anti-plasmodial drugs. High-throughput screening is an efficient and relatively fast method to screen potential anti-plasmodial compounds for the ability to prevent the crystallization of heme to hemozoin. An automated high-throughput screening method is being developed to test for potential anti-plasmodial activity in a number of natural products.

NP-03 **Ella Cortinas[1,2], Cynthia Grim[1,2]**, Emily Trebour[1,2], Timothy Geary[3], Vicki Muise[3], Bill J. Baker[1,2].
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[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 cerevisae 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 4,000 crude extracts from various fungal and bacterial sources, as well as, 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 from developing drug resistance .

NP-04 **Alex Cole[1,2]**, Jacqueline von Salm[1,2], Bill J. Baker[1,2].
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Evidence of Bioactive Punaglandins Found in Coral at Clearwater Beach, Florida

Much like prostaglandins, halogenated punaglandins have been shown to have anti-inflammatory and antitumor activity. The soft coral, Telesto riisei, previously collected in Hawaii, was found to contain highly functionalized punaglandis. T. riisei was recently collected in Clearwater Beach, Florida and appears to demonstrate similar chemistry as those previously studied despite considerable variation in respective ecosystems. The dichloromethane extract was separated and purified in a series of chromatographic methods monitored via 1H-NMR guided fractionation. Isolated compounds will be compiled in the Chemodiversity lab's chemical library at the University of South Florida's Center for Drug Discovery and Innovation in order to screen them against a number of bioassays including neglected diseases such as Leishmaniasis and the ESKAPE pathogens. Due to the variation in habitat amongst the coral samples, there is also the possibility of extracting novel compounds within the samples collected at Clearwater Beach FL.

NP-05 **Riley Bednar[1,2], Evan O'Sullivan[1,2], Roger Stern[1,2]**, Christopher Witowski[1,2], Bill J. Baker[1,2].
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Solid-State Co-culturing of Bipolaris sp. Leads to a New Malformin Peptide

Secondary metabolites are an invaluable reservoir for pharmaceutical compounds, particularly for new antibiotic leads. Competition for resources among organisms elicits the production of secondary metabolites as a defensive measure to ward off antagonists, leading to the induction of biosynthetic pathways that may yield titer enhancement of metabolites, or to the production of new secondary metabolites. This study demonstrates that solid-state co-culturing with Aspergillus niger and a Bipolaris sp. fungus from a Xestospongia muta sponge, can elicit the production of new secondary metabolites. Structure elucidation reveals production of a new analogue of the malformins, by the Bipolaris fungus. Malformins are a class of cytotoxic secondary metabolites, structurally defined as cyclic pentapeptides of varying D/L stereochemistry with a sulfur bridge, associated with Aspergillus sp.

Further chromatographic analysis with Marfey's reagent also reveals that one of the isolated malformins contains an uncharacterized stereochemistry around its isoleucine residue, constituting a new secondary metabolite.

NP-06 **Roxanna Gould[1], Abigail Lee[1]**, Michael Veri[1], Bill J. Baker[1,2].
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Compound Isolation and Structural Elucidation From Marine Sources

Natural products chemistry, which offers a wealth of chemicals already tailored by evolution for activity in biological systems, is a rich source for novel compound discovery. Following extraction, compounds exist in complex mixtures; these mixtures must be separated into individual compounds, which can then be identified.

NP-07 **Deniz Hay[1,2], Micheal O'Donnell[1,2]**, Chris Witowski[1,2], Laurent Calcul[2], Bill J. Baker[1,2].
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High-Throughput Screening of Marine Microorganisms for Discovery of Anti-Infectives

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. The particular research interest in this project involves the isolation of bioactive compounds obtained from small-scale liquid cultures of marine microorganisms collected from algae, coral, sponges, mangroves and tunicates. Microbes of interest are subjected to epigenetic modification during cultivation in order to stimulate an increase in the production of secondary metabolites. Fractions are prepared from extracts with automated liquid chromatography-mass spectrometry (LC-MS) for high-throughput screening targeting activity against the Leishmaniasis causing parasite Leishmania donovani and the drug-resistant ESKAPE bacteria. This project will highlight initial methodology, bioactivity profiles and preliminary metabolomic data on active fractions.

NP-08 **Shane Clark[1,2]**, Christopher Witowski[1,2], Jacqueline von Salm[1,2], Bill J. Baker[1,2].
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The Chemotypic properties of Distaplia Stylifera and Diplosoma Listerianum

Natural products have benefited modern medicine with bioactive molecules and therapeutic medicines. Marine organisms have offered a wide array of compounds to this field. Tunicates are sessile marine organisms which produce secondary metabolites as a self-defense from predication. Secondary metabolites are biological compounds that are not essential to the organism's growth, development, or reproduction that have been specialized through evolution, to support and protect the organism. Six samples, containing two genera of tunicates, Distaplia Stylifera and Diplosoma Listerianum were collected from Clearwater Reef, FL for metabolomics screening. These tunicates have yet to be studied in the Gulf of Mexico, hence the need for chemical analysis. Therefore, these tunicates have been extracted and analyzed with liquid chromatography- mass spectrometry (LC-MS) and gas chromatography- mass spectrometry (GC-MS). The metabolic profiles will be analyzed within the samples and bioactivity of the extracts will be explored.

NP-09 **Eno-emem Okpokpo[1,2]**, Danielle Demers[1,2], Matthew Knestrick[1,2], Renee Fleeman[3], Lindsey N. Shaw[3], Bill J. Baker[1,2].
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Epigenetic Modification of Mangrove Endophytic Fungal Species for the Purpose of Drug Discovery against the ESKAPE Pathogens

In drug discovery, natural products have shown great promise, with about 71% of drugs approved between 1981 and 2010. Mangrove endophytic fungi are of great interest in the study of natural product isolation. Considering that these organisms are grown away from their natural habitat, their metabolic processes tend to differ to some degree. Therefore, their growth conditions have to be modified to encourage the production of metabolites that would probably not be observed otherwise. After the modification process, the fungal samples are extracted and screened against the multi-drug resistant ESKAPE pathogens. The organism whose extract shows activity against the ESKAPE pathogens is then grown in larger scale so as to obtain the metabolite responsible for the antimicrobial properties. A dereplication process is very important to avoid finding already known compounds. The work presented herein shows the natural product dereplication process following the identification of a "hit" sample.

NP-10 **Chelsea Fugate[1,2], Alexa Pullicin[1,2], Lindsay Vacca[1,2], Ariel Watts[1,2],** Danielle Demers[1,2], Matthew Knestrick[1,2], Renee Fleeman[3], Lindsey N. Shaw[3], Bill J. Baker[1,2].
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Epigenetic Modification of Endophytic Fungi

Drug resistance among bacterial pathogens is increasing steadily due to factors such as transposons and resistance genes being exchanged between bacteria. Drug discovery for new antibacterial elements is declining, creating a great need for new antibiotics. The ESKAPE pathogens, a panel of six drug resistant, clinically relevant bacteria, are an ideal target for drug discovery screening. Endophytic fungi isolated from mangroves are extracted and screened against these pathogens in a medium-throughput drug discovery screening effort. Epigenetic modification is used during the culture process to help identify new and novel active compounds. Epigenetic modification serves to uncover previously down-regulated or silent biosynthetic pathways, revealing their true biosynthetic potential. The fungal extracts are submitted for an MIC bioassay against all of the ESKAPE pathogens. Organisms that produce extracts that have bacteriocidal or bacteriostatic properties will be scaled-up and the active molecule isolated and identified.

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Selected Components Subtractive Chromatography from Camellia Sinensis for Brain Health Effect Evaluation

The leaves of the Chinese plant, Camellia sinensis have been used as traditional Chinese medicine for thousands of years and the resulting hot evening beverage from its leaves and leaf buds became popular as green tea. The USF Botanical Gardens provided green tea powder, rich in polyphenol compounds that may affect brain health. The boiling water extract from the powder of Camellia sinensis was subjected to a subtractive chromatographic separation using preparative LC-MS at the Center of Excellence for Drug Discovery and Innovation (CDDI) Chemodiversity Facility which produced two fractions (fraction A as the selected subtracted major components and fraction B as the corresponding remaining extract). The resulting pairs of subtractive chromatographied fractions will be submitted to the College of Molecular Medicine and the Center of Excellence for Aging and Brain Repair to evaluate the bioactivity contribution of to examine the anti-inflammatory actions and prevention of reactive oxygen species production.

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Natural Products Drug Discovery Screening Against Leishmania sp.

Leishmaniasis is a Neglected Tropical Disease caused by a protozoa (Leishmania sp.) and transmitted by a sandfly. This disease can be fatal, and resists most treatments that are available. Natural products have played an important role in drug discovery; around 2/3 of drugs on the market today can be traced back to natural products. Therefore, a natural products based drug discovery screening project has been undertaken against the parasite. A library of mangrove endophytic fungi, isolated from the Florida coast, is being cultured in an attempt to isolate compounds for the treatment of this disease. Fungi are cultured under various conditions to elicit maximum expression of secondary metabolites, extracted, and the extracts are then screened against the parasite and for cytotoxicity. Organisms that produce activity against the parasite will be extracted, and have their active compound(s) elucidated. This presentation will be a progress report on the samples screened to date.

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Further Chemical Investigation from the 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 goal is 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

will be added to the unique Natural Products library of the Center of Excellence for Drug Discovery and Innovation (CDDI) Chemodiversity Facility.

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Probing Secondary Metabolites from Octocoral Briareum Asbestinum

Anthozoan coral B. asbestinum is a main source of 2-11 cyclized cembranoids, a class of diterpenes of which several subclasses have been found to be promising as drug precursors due to their varied antiviral and cytotoxic activities. In an effort to contribute to the chemical diversity library at the Center of Excellence for Drug Discovery and Innovation (CDDI), B. asbestinum was soxhlet extracted in methylene chloride and fractionated via medium pressure liquid chromatographic (MPLC). Resulting UV-active fractions were purified by high performance liquid chromatography (HPLC), and their corresponding sub-fractions were analyzed by NMR and mass spectrometry. Resulting data will allow the characterization of secondary metabolites present.